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PATENT- OG VAREMÆRKESTYRELSEN

SUBTILASES

FIELD OF THE INVENTION

The present invention relates to JP170 and BPN' like subtilases and to methods of construction such variants with altered properties, such as stability (e.g. thermostability or storage stability), Ca^{2+} dependency, pH dependent activity, improved performance in washing and cleaning applications.

BACKGROUND OF THE INVENTION

Enzymes have been used within the detergent industry as part of washing formulations for more than 30 years. Proteases are from a commercial perspective the most relevant enzyme in such formulations, but other enzymes including lipases, amylases, cellulases or mixtures of enzymes are also often used.

To improve the cost and/or the performance of proteases there is an ongoing search for proteases with altered properties, such as increased activity at low temperatures, increased thermostability, increased specific activity at a given pH, altered Ca^{2+} dependency, increased stability in the presence of other detergent ingredients (e.g. bleach, surfactants etc.) etc.

The search for proteases with altered properties include both discovery of naturally occurring proteases, i.e. so called wild-type proteases but also alteration of well-known proteases by e.g. genetic manipulation of the nucleic acid sequence encoding said proteases. Knowledge of the relationship between the three-dimensional structure and the function of a protein has improved the ability to evaluate which areas of a protein to alter to affect a specific characteristic of the protein.

One family of proteases, which are often used in detergents, are the subtilases. This family has previously been further grouped into 6 different sub-groups by Siezen RJ and Leunissen JAM, 1997, Protein Science, 6, 501-523. One of these sub-groups is the Subtilisin family which includes subtilases such as BPN', subtilisin 309 (SAVINASE®, NOVOZYMES A/S), subtilisin Carlsberg (ALCALASE®, NOVOZYMES A/S), subtilisin S41 (a subtilase from the psychrophilic Antarctic *Bacillus* TA41, Davail S et al. 1994, The Journal of Biological Chemistry, 269(26), 99. 17448-17453), subtilisin S39 (a subtilase from the psychrophilic Antarctic *Bacillus* TA39, Narinx E et al. 1997, Protein Engineering, 10 (11), pp. 1271-1279) and TY145 (a subtilase from Bacillus sp. TY145, NCIMB 40339 described in WO 92/17577).

However, despite the sequence homology between the subtilases belonging to the Subtilisin subgroup of subtilases, modelling of the three-dimensional structure of one subtilase

on the basis of the three-dimensional structure of another subtilase may result in an incorrect three-dimensional model structure because of structural differences.

Recently the three-dimensional structure of subtilase TY145 have been elucidated and it was found that there are several differences between this and the three-dimensional structure of BPN' also belonging to the Subtilisin subgroup of subtilases (Danish application PA 2003 00119).

The differences between the three-dimensional structures of TY145 and BPN' are confirmed by the three-dimensional structure of the subtilase "sphericase" from *Bacillus sphaericus* (PDB NO:1EA7, Protein Data Bank). The overall structure and many details of this subtilase are very homologous with the TY145 subtilase structure.

Now the inventors of the present invention disclose the three-dimensional structure of the subtilase JP170. This subtilase also has great structural differences compared to BPN' and TY145.

The subtilase JP170 and subtilases similar to JP170 are already known in the art, but the three-dimensional structure of the present invention has not been disclosed for such subtilases.

The JP170 subtilase was first described as protease A in WO 88/01293 to Novo Nordisk. Later the patent application WO 98/56927 to Novo Nordisk Biotech disclosed the amino acid (polypeptide) sequence of JP170 and the DNA sequence encoding JP170. The patents JP7-62152 and JP 4197182 to Lion Corp. disclosed the alkaline app. 46 kD protease Y produced by *Bacillus sp.* Y that is homologous to JP170 and the DNA sequence encoding protease Y. And in addition US 6,376,227 to Kao Corp. discloses physical characteristics as well as DNA and polypeptide sequences of alkaline proteases KP43, KP1790 and KP9860 which are also homologous to JP170. Recently variants of the KP43, KP9860, SD-521 and Y proteases among others were disclosed in EP 1209233. These variants have the accession numbers aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081, aam50080. These proteases are highly homologous, and an alignment of KP43, KP9860, SD-521, Y and JP170 revealed at least 90% homology. Therefore JP170, Y (aay44619) and SD-521 (aam50084) represent these proteases in the alignments of the present application.

In the literature, modelling based on three-dimensional structures of proteins has been used to transfer advantageous properties from one protein to another. Miyazaki K et al.

2000, J Mol Biol, 297, pp.1015-1026 discloses enhancement of the thermostability and activity of the psychrophilic protease subtilisin S41 by methods of directed evolution.

Wintrode TL et al. 2000, Journal of Biological Chemistry, 275 (41), pp. 31635-31640 discloses conversion of a mesophilic subtilisin-like protease from *Bacillus sphaericus* SSII into its psychrophilic counterpart by methods of directed evolution. Wintrode et al. constructed the three-dimensional structural model of the SSII subtilase on basis of its homology with subtilisins Carlsberg, Savinase, BPN' and Thermitase, but according to the disclosure of the three-dimensional structure of the TY145 subtilase, the SSII subtilase pertain to the new group of TY145 like subtilases.

BRIEF DESCRIPTION OF THE INVENTION

The inventors have modified the amino acid sequence of a subtilase to obtain variants with improved properties, based on the three-dimensional structure of the subtilases JP170 and BPN'. The variants have altered properties, such as increased activity at low temperatures, increased thermostability, increased specific activity at a given pH, altered Ca^{2+} dependency, increased stability in the presence of other detergent ingredients (e.g. bleach, surfactants etc.) etc.

Accordingly, the object of the present invention is to provide a method for constructing subtilases having altered properties, in particular to provide a method for constructing subtilases having altered properties as described above.

Thus, in its broadest aspect, the present invention relates to a method for constructing a variant of a parent subtilase, wherein the variant has at least one altered property as compared to said parent subtilase, which method comprises:

i) analyzing the three-dimensional structure of the subtilase to identify, on the basis of an evaluation of structural considerations, at least one amino acid residue or at least one structural region of the subtilase, which is of relevance for altering said property;

ii) constructing a variant of the subtilase, which as compared to the parent subtilase, has been modified in the amino acid residue or structural part identified in i) so as to alter said property; and

iii) testing the resulting subtilase variant for said property.

Although it has been described in the following that modification of the parent subtilase in certain regions and/or positions is expected to confer a particular effect to the thus produced subtilase variant, it should be noted that modification of the parent subtilase in any of such regions may also give rise to any other of the above-mentioned effects. For example,

any of the regions and/or positions mentioned as being of particular interest with respect to, e.g., improved thermostability, may also give rise to, e.g., higher activity at a lower pH, an altered pH optimum, or increased specific activity, such as increased peptidase activity.

Further aspects of the present invention relates to variants of a subtilase, the DNA encoding such variants and methods of preparing the variants. Still further aspects of the present invention relates to the use of the variants for various industrial purposes, in particular as an additive in detergent compositions. Other aspects of the present invention will be apparent from the below description as well as from the appended claims.

BRIEF DESCRIPTION OF FIGURES AND APPENDIX

Figure 1, Alignment of 3D sequences of protease JP170 (mature sequence from Appendix 1), SD-521 (aam50084 from EP 1209233) and protease Y (aay44619 from WO99/67370). By 3D sequences is meant that the position of homologous residues are chosen by superposition of the 3D structures and subsequently the amino acid sequences are aligned based on these homologous positions.

Figure 2, Superposition of JP170 and Savinase 3D structures, with indication of calcium binding sites. JP170: light structure and three ion-binding sites. Savinase: dark structure and two ion-binding sites.

Figure 3, Matrix of homology between subtilases pertaining to the JP170 and BPN' subgroups. The sequences are identified by sequence database accession numbers.

APPENDIX 1 shows the structural coordinates for the solved crystal structure of JP170.

DEFINITIONS

Prior to discussing this invention in further detail, the following terms and conventions will first be defined.

For a detailed description of the nomenclature of amino acids and nucleic acids, we refer to WO 00/71691 page 5, hereby incorporated by reference. A description of the nomenclature of modifications introduced in a polypeptide by genetic manipulation can be found in WO 00/71691 page 7-12, hereby incorporated by reference.

The term "subtilases" refer to a sub-group of serine protease according to Siezen *et al.*, *Protein Engng.* 4 (1991) 719-737 and Siezen et al. *Protein Science* 6 (1997) 501-523. Ser-

ine proteases or serine peptidases is a subgroup of proteases characterised by having a serine in the active site, which forms a covalent adduct with the substrate. Further the subtilases (and the serine proteases) are characterised by having two active site amino acid residues apart from the serine, namely a histidine and an aspartic acid residue.

Subtilases are defined by homology analysis of more than 170 amino acid sequences of serine proteases previously referred to as subtilisin-like proteases. The subtilases may be divided into 6 sub-divisions, i.e. the Subtilisin family, the Thermitase family, the Proteinase K family, the Lantibiotic peptidase family, the Kexin family and the Pyrolysin family.

The Subtilisin family (EC 3.4.21.62) may be further divided into 3 sub-groups, i.e. I-S1 ("true" subtilisins), I-S2 (highly alkaline proteases) and intracellular subtilisins. Definitions or grouping of enzymes may vary or change, however, in the context of the present invention the above division of subtilases into sub-division or sub-groups shall be understood as those described by Siezen et al., *Protein Engng.* 4 (1991) 719-737 and Siezen et al. *Protein Science* 6 (1997) 501-523.

The term "parent" is in the context of the present invention to be understood as a protein, which is modified to create a protein variant. The parent protein may be a naturally occurring (wild-type) polypeptide or it may be a variant thereof prepared by any suitable means. For instance, the parent protein may be a variant of a naturally occurring protein which has been modified by substitution, chemical modification, deletion or truncation of one or more amino acid residues, or by addition or insertion of one or more amino acid residues to the amino acid sequence, of a naturally-occurring polypeptide. Thus the term "parent subtilase" refers to a subtilase which is modified to create a subtilase variant.

The term "variant" is in the context of the present invention to be understood as a protein which has been modified as compared to a parent protein at one or more amino acid residues.

The term "modification(s)" or "modified" is in the context of the present invention to be understood as to include chemical modification of a protein as well as genetic manipulation of the DNA encoding a protein. The modification(s) may be replacement(s) of the amino acid side chain(s), substitution(s), deletion(s) and/or insertions in or at the amino acid(s) of interest. Thus the term "modified protein", e.g. "modified subtilase", is to be understood as a protein which contains modification(s) compared to a parent protein, e.g. subtilase.

The term "JP170 subtilase" or "JP170 like subtilase" should in the context of the present invention be understood as a subtilase belonging to the Subtilisin group according to Siezen et al. *Protein Science* 6 (1997) 501-523 and which has at least 58% homology to JP170 SEQ ID NO:1. Thus, among others the alkaline proteases KP43, KP1790, KP9860, Y and SD-521 are subtilases belonging to the JP170 subgroup of subtilases. In the context of the present invention a JP170 subtilase has three ion-binding sites. However, the number of ion-binding sites may vary in similar structures depending on the medium used for crystallisation. It appears e.g. that two of five ion-binding sites of *Bacillus sphaericus* "sphericase" (PDB NO:1EA7, Protein Data Bank) were due to a calcium containing crystallisation medium.

The term "(a) BPN' subtilase" or "(a) BPN' like subtilase" should in the context of the present invention be understood as a subtilase belonging to the Subtilisin group according Siezen et al. Siezen et al. *Protein Science* 6 (1997) 501-523 and which has at least 61% homology to BPN' SEQ ID NO:5. Such a BPN' like subtilase is for example Savinase. In the context of the present invention a BPN' subtilase has two ion-binding sites. A BPN' like subtilase may, in the context of the present invention, belong to branch I-S of the subtilisins i.e. to branch I-S1, the "true" subtilisins or I-S2, the highly alkaline proteases (Siezen et al., *Protein Engng.* 4 (1991) 719-737).

"Homology" or "homologous to" is in the context of the present invention to be understood in its conventional meaning and the "homology" between two amino acid sequences should be determined by use of the "Similarity" defined by the GAP program from the University of Wisconsin Genetics Computer Group (UWGCG) package using default settings for alignment parameters, comparison matrix, gap and gap extension penalties. Default values for GAP penalties, i.e. GAP creation penalty of 3.0 and GAP extension penalty of 0.1 (Program Manual for the Wisconsin Package, Version 8, August 1994, Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA 53711). The method is also described in S.B. Needleman and C.D. Wunsch, Journal of Molecular Biology, 48, 443-445 (1970). Identities can be extracted from the same calculation. The homology between two amino acid sequences can also be determined by "identity" or "similarity" using the GAP routine of the UWGCG package version 9.1 with default setting for alignment parameters, comparison matrix, gap and gap extension penalties can also be applied using the following parameters: gap creation penalty = 8 and gap extension penalty = 8 and all other parameters kept at their default values. The output from the routine is besides the amino acid alignment the

calculation of the "Percent Identity" and the "Similarity" between the two sequences. The numbers calculated using UWGCG package version 9.1 is slightly different from the version 8.

The term "position" is in the context of the present invention to be understood as the number of an amino acid in a peptide or polypeptide when counting from the N-terminal end of said peptide/polypeptide. The position numbers used in the present invention refer to different subtilases depending on which subgroup the subtilase belongs to.

As mentioned above the alkaline subtilases KP43, KP1790, KP9860, Y, SD-521 and variants aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081, aam50080 of EP 1209233 belong to the JP170 subgroup, based on sequence homology. Due to the extensive homology only subtilase Y and SD-521 are aligned with JP170. The Y subtilase and SD-521 subtilase are numbered according to SEQ ID NO:2 and 3 respectively.
Likewise other subtilases belonging to the JP170 subgroup are numbered individually according to their own sequence. However in order to determine homologous positions in such other subtilases an alignment with the each of SEQ ID's NO:1, 2 and 3 is conducted according to the GAP procedure described above. Subsequently the homologous positions are determined with reference to the most homologous of SEQ ID's NO:1, 2 and 3.

Alternatively subtilases belonging to the JP170 subgroup can be numbered by reference to the positions of JP170 subtilase (SEQ ID NO:1).

Subtilases belonging to the BPN' subgroup refers to the positions of Subtilisin Novo (BPN') from *B. amyloliquefaciens*.

DETAILED DESCRIPTION OF THE INVENTION

Despite the great homology of the subtilases described above the inventors of the present invention have elucidated the three-dimensional structure of JP170, SEQ ID NO:1 by X-ray crystallography and found that there are several differences between this and the three-dimensional structure of BPN'. The inventors of the present invention have further compared the sequence homology of subtilases belonging to the Subtilisin subgroup. This is shown in Figure 3 of the present invention.

On the basis of this comparison the inventors of the present invention suggest to divide the Subtilisin subgroup so that the JP170 subtilases become a separate subgroup in addition to the subgroups of BPN' subtilases and TY145 subtilases (DKPTO, PA 2003 00119).

JP170 subtilases

As described above a JP170 like subtilase is in the context of the present invention to be understood as a subtilase which has at least 58% homology to SEQ ID NO:1. In particular said JP170 subtilase may have at least 60% homology to SEQ ID NO:1, such as at least 65%, at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to JP170, i.e. to SEQ ID NO:1.

In a first embodiment of the present invention a JP170 subtilase suitable for the purpose described herein may be a subtilase homologous to the three-dimensional structure of JP170, i.e. it may be homologous to the three-dimensional structure defined by the structure coordinates in Appendix 1.

As it is well-known to a person skilled in the art that a set of structure coordinates for a protein or a portion thereof is a relative set of points that define a shape in three dimensions, it is possible that an entirely different set of coordinates could define an identical or a similar shape. Moreover, slight variations in the individual coordinates may have little or no effect on the overall shape.

These variations in coordinates may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates of JP170 (Appendix 1) may be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above. Alternatively, said variations may be due to differences in the primary amino acid sequence.

If such variations are within an acceptable standard error as compared to the structure coordinates of Appendix 1 said three-dimensional structure is within the context of the present invention to be understood as being homologous to the structure of Appendix 1. The standard error may typically be measured as the root mean square deviation of e.g. conserved backbone residues, where the term "root mean square deviation" (RMS) means the square root of the arithmetic mean of the squares of the deviations from the mean.

As it is also well-known to a person skilled in the art that within a group of proteins which have a homologous structure there may be variations in the three-dimensional structure in certain areas or domains of the structure, e.g. loops, which are not or at least only of a small importance to the functional domains of the structure, but which may result in a big root mean square deviation of the conserved residue backbone atoms between said structures.

Thus it is well known that a set of structure coordinates is unique to the crystallised protein. No other three dimensional structure will have the exact same set of coordinates, be it a homologous structure or even the same protein crystallised in different manner. There are natural fluctuations in the coordinates. The overall structure and the inter-atomic relationship can be found to be similar. The similarity can be discussed in terms of root mean square deviation of each atom of a structure from each "homologous" atom of another structure. However, only identical proteins have the exact same number of atoms. Therefore, proteins having a similarity below 100% will normally have a different number of atoms, and thus the root mean square deviation can not be calculated on all atoms, but only the ones that are considered "homologous". A precise description of the similarity based on the coordinates is thus difficult to describe and difficult to compute for homologous proteins. Regarding the present invention, similarities in 3D structure of different subtilases can be described by the content of homologous structural elements, and/or the similarity in amino acid or DNA sequence. For sequences having no deletions or insertions a RMS for the calcium atoms can be calculated.

Examples of JP170 like subtilases include the alkaline proteases KP43, KP1790, KP9860, Y, SD-521 and variants aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081, aam50080 of EP 1209233, however to the best of our knowledge the three-dimensional structure has not been solved for any of these subtilases.

Accordingly, a preferred embodiment of the present invention is a parent subtilase or a subtilase variant which is at least 58% homologous to the sequence of SEQ ID NO:1, preferably at least 60, at least 65%, at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homologous to the sequence of SEQ ID NO:1, and optionally said subtilase further comprises the following structural characteristics:

a) a twisted beta-sheet with 7 strands,

b) six alpha helices,

c) three ion-binding sites and

not comprising the Strong and Weak ion-binding site of the BPN' like subtilases, and with the exception of the subtilases JP170, KP1790, KP9860, KP43, Y, SD-521 and variants aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081, aam50080 of EP 1209233.

The JP170 subtilase of the present invention is encoded by an isolated nucleic acid sequence, which nucleic acid sequence encodes a subtilase which has at least 58% homology to SEQ ID NO:1. In particular said nucleic acid sequence encodes a subtilase that has at least 60% homology to SEQ ID NO:1, such as at least 65%, at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to SEQ ID NO:1, i.e. to the amino acid sequence of JP170.

Further the isolated nucleic acid sequence encoding a JP170 subtilase of the invention hybridizes with a complementary strand of a nucleic acid sequence encoding the amino acid sequence of SEQ ID NO:1 preferably under low stringency conditions, at least under medium stringency conditions, at least under medium/high stringency conditions, at least under high stringency conditions, at least under very high stringency conditions.

Suitable experimental conditions for determining hybridization at low, medium, or high stringency conditions between a nucleotide probe and a homologous DNA or RNA sequence involves presoaking of the filter containing the DNA fragments or RNA to hybridize in 5 x SSC (Sodium chloride/Sodium citrate, Sambrook et al. 1989) for 10 min, and prehybridization of the filter in a solution of 5 x SSC, 5 x Denhardt's solution (Sambrook et al. 1989), 0.5 % SDS and 100 µg/ml of denatured sonicated salmon sperm DNA (Sambrook et al. 1989), followed by hybridization in the same solution containing a concentration of 10ng/ml of a random-primed (Feinberg, A. P. and Vogelstein, B. (1983) *Anal. Biochem.* 132:6-13), ^{32}P-dCTP-labeled (specific activity > 1 x 10^9 cpm/µg) probe for 12 hours at ca. 45°C. The filter is then washed twice for 30 minutes in 2 x SSC, 0.5 % SDS at least * 55°C (low stringency), more preferably at least 60°C (medium stringency), still more preferably at least 65°C (medium/high stringency), even more preferably at least 70°C (high stringency), and even more preferably at least 75°C (very high stringency).

BPN' subtilases

As described above a BPN' subtilase is in the context of the present invention to be understood as a subtilase which has at least 61% homology to SEQ ID NO:4. In particular said BPN' subtilase may have at least 65%, such as at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to BPN', i.e. to SEQ ID NO:4.

In one embodiment of the present invention a BPN' subtilase suitable for the purpose described herein may be a subtilase homologous to the three-dimensional structure of BPN' as defined by the structure coordinates given in PDB Nos. 1SBT and 1GNS (Protein Data Bank), or one of the several other structures of BPN' that are accessible from the Protein Data Bank. Variations between homologous structures may occur for several reasons as described above. Thus a BPN' subtilase within the context of the present invention is to be understood as any subtilase having the structural characteristics pertaining to the BPN' subtilases as described above, and in addition such subtilases does preferably not have further structural characteristics which are not present in the BPN' subtilases as described herein. Further a BPN' subtilase of the present invention may have the necessary percentage of similarity with SEQ ID NO:4.

Examples of BPN' like subtilases include the subtilisin 309 (PDB NO:1SVN, SAVINASE®, NOVOZYMES A/S) and subtilisin Carlsberg (ALCALASE®, NOVOZYMES A/S), among others.

In figure 1 of R.J. Siezen and J.A.M Leunissen (Protein science, Vol. 6 (3), pp. 501-523, 1997) page 502 a structure of subtilases is described. A subtilase consists of 6-8 helices, 11 strands of which 7 are central in a twisted beta-sheet. Two ion-binding sites are mentioned, the so called "Strong" and "Weak" calcium-binding sites. It was later discovered that for some structures (subtilisin DY PDB no. 1BH6, 1998), the Weak calcium-binding site was shown to be a Na (sodium) binding site when the calcium concentration in the crystallization medium was low. Thus, in the following we refer to ion-binding sites instead of calcium-binding sites.

The BPN' subtilase of the present invention is encoded by an isolated nucleic acid sequence, which nucleic acid sequence encodes a subtilase which has at least 61% homology to SEQ ID NO:4. In particular said BPN' subtilase may have at least 65%, such as at

least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 91%, at least 92%, at least 93%, at least 94%, at least 95%, at least 96%, at least 97%, at least 98% or at least 99% homology to BPN', i.e. to SEQ ID NO:4.

Further the isolated nucleic acid sequence encoding a BPN' subtilase of the invention hybridizes with a complementary strand of the nucleic acid sequence encoding the amino acid sequence of SEQ ID NO:4 preferably under low stringency conditions, at least under medium stringency conditions, at least under medium/high stringency conditions, at least under high stringency conditions, at least under very high stringency conditions.

Three-dimensional structure of JP170 subtilases

The JP170 subtilase was used to elucidate the three-dimensional structure forming the basis for the present invention.

The structure of JP170 was solved in accordance with the principle for x-ray crystallographic methods, for example, as given in X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989.

The structural coordinates for the solved crystal structure of JP170 are given in standard PDB format (Protein Data Bank, Brookhaven National Laboratory, Brookhaven, CT) as set forth in Appendix 1. It is to be understood that Appendix 1 forms part of the present application. In the context of Appendix 1, the following abbreviations are used: CA refers to c-alpha (carbon atoms) or to calcium ions, (however to avoid misunderstandings we use the full names "c-alpha atoms" and "calcium" or "ion" in the present specification). Amino acid residues are given in their standard three-letter code. The attached structural coordinates contain the protease structure, and an inhibitor structure CI2 as well as water molecules. The protease coordinates has a chain identification called A, whereas the CI2 inhibitor is called B, the calcium ions are called C, and the water is W. In the following the positions of the mentioned residues refer to the sequence of JP170 as disclosed in SEQ ID NO:1.

The JP170 structure consists of two domains, a catalytic domain and a C-terminal domain. The structure of the catalytic domain shows the same overall fold as found in the S8 family of subtilisins. The structure comprises a twisted beta-sheet with 7 strands arranged in the following sequential order S2, S3, S1, S4, S5, S6, S7.

There are six alpha helices in the catalytic domain structure of which number H1 contains residues 9-17, H2 contains residues 68-76, H3 contains residues 110-119, H4 contains residues 139-150, H5 contains residues 253-273 and H6 contains residues 281-291.
The C-terminal domain comprises a strand motif, a so called "beta sandwich" consisting of sheets a and b. The sheet in this domain is combined of strands in an anti-parallel fashion, whereas the strand in the catalytic domain is combined in parallel. The sequential order of the strands can be denoted as: S1a-S1b-S3a-S3b-S4b-S4a-S2b-S2a with the beta sandwich organised as to the two sheets S1a, S3a, S4a, S2a and S1b, S3b, S4b, S2b.

The JP170 subtilases are shown to lack the well-known Strong and Weak ion-binding sites of the BPN' subtilases. However, the JP170 subtilases have three ion-binding sites which are not present in the BPN' subtilisin structures. This can be seen in the structural alignment presented in Figure 2. These three ion-binding sites are hereinafter referred to as Site 1, which is placed in the catalytic domain, and Site 2 and 3 which are placed in the non-catalytic C-terminal domain.

Thus in relation to the atomic coordinates disclosed in Appendix 1, the ion-binding sites of JP170 are located at:
Site 1 - calcium atom named A601 CA
Site 2 - calcium atom named A603 CA, and
Site 3 - calcium atom named A602 CA in the PDB table (Appendix 1).

The position of an ion-binding site can be defined by the distance to four specific atoms in the core structure. The distance from the ion-binding site to the c-alpha atoms of the three active site residues has been chosen. Throughout the subtilases the residues Ser, His and Asp in the active site are highly conserved. In JP170 they are Asp30, His68 and Ser254. The fourth distance chosen is the distance to the c-alpha atom of the amino acid residue coming first after the active site serine residue in the sequence (herein after called "next to Ser"); in the 3D structure of JP170 it is Met255.
In a preferred embodiment of the present invention, the distance between:

a) ion-binding site 1 and i) Asp c-alpha atom is 26.70-28.70Å, ii) His c-alpha atom is 22.10-24.10Å, iii) Ser c-alpha atom is 16.95-18.95Å, iv) next to Ser c-alpha atom is 15.30-17.30Å,
b) ion-binding site 2 and i) Asp c-alpha atom is 33.50-35.50Å, ii) His c-alpha atom is 37-39Å, iii) Ser c-alpha atom is 29.40-31.40Å, iv) next to Ser c-alpha atom is 30.70-

32.70Å,

c) ion-binding site 3 and i) Asp c-alpha atom is 41.50-43.50Å, ii) His c-alpha atom is 42.90-44.90Å, iii) Ser c-alpha atom is 34.50-36.50Å, iv) next to Ser c-alpha atom is 35-37Å.

Below are the specific distances between the four chosen c-alpha atoms and the three ion binding sites of the JP170 subtilase given in Å:

	site 1	site 2	site 3
Met255	16.34	31.68	36.02
His68	23.12	38.03	43.87
Asp30	27.69	34.49	42.48
Ser254	17.95	30.41	35.51
site 1	0	35.29	32.92
site 2	35.29	0	14.08
site 3	32.92	14.08	0

However these distances may vary from one subtilase to the other. The present distances are given with a calcium ion in the structure. If a sodium ion was bound instead the distances would be shifted a little bit. Generally the distances can vary ±0.80Å, preferably ±0.70Å, ±0.60Å, ±0.50Å, ±0.40Å, or most preferably ±0.30Å.

Further, in the JP170 like subtilases, the peptide structure circumventing ion-binding site 1 up to a distance of 10 Å is composed of the amino acid residues placed in positions 183-189, 191-204 and 224-225.

The peptide structure circumventing ion-binding site 2 up to a distance of 10 Å is composed of residues 378-393.

The peptide structure circumventing ion-binding site 3 up to a distance of 10 Å is composed of residues 348, 350, 352, 363-370, 380-383, 391-400 and 414-420.

In comparison with the BPN' like subtilase structures the structure of the JP170 like subtilases can be divided into a "core subtilase-like" region, an "intermediate" region and a "nonhomologous" region.

The active site can be found in the core subtilase-like region, which is structurally closely related to the BPN' structures. The core subtilase-like region is composed of residues 17-34, 197-209 and 216-232, and contains the alpha-helix H3 and the central alpha-helix H5 in

which the active site serine residue is situated in the N-terminal part. The core subtilase-like region has an RMS lower than 1.2.
Outside the core subtilase-like region the structure of the JP170 like subtilase differs from the BPN' structures to a greater extent.

The intermediate region consists of residues 42-46, 150-186, 245-272 and 278-296. The intermediate region has an RMS bigger than 1.2 and less than 1.8. The relationships between the three-dimensional structure and functionality are potentially difficult to predict in this region of the JP170 like subtilases.

The nonhomologous region consists of residues 1-16, 35-41, 47-149, 187-196, 210-215, 233-244, 273-277 and 297-316. The nonhomologous region has a RMS higher than 1.8. The relationships between the three-dimensional structure and functionality are very difficult to predict in this region of the JP170 like subtilases.

Many loops in the 3D structure of the JP170 like subtilases differ significantly from the BPN' type structures, both in length and in content of amino acid residues. The following loops or protein sequence stretches of JP170 are compared to Savinase (in parenthesis):
G32-H43 (G34-H39)
E44-Y54 (P40-A48)
G57-G67 (V51-G63)
N79-N82 (I75-V81)
I96-P107 (V95-S105)
A108-S119 (106-N117)
A131-Y137 (S128-S132)
T138-D152 (A133-G146)
E162-I169 (S156-I165)
G173-T180 (A169-A176)
E185-N199 (D181-N184)
G208-D218 (G193-D197)
S232-K246 (G211-T213)
D294-N303 (S256-L262)

The loops N79-N82 (I75-V81) and G208-D218 (G193-D197) are in contact with a ion-binding site in Savinase, but not in JP170. Similarly the loop E185-N199 (D181-N184) is in

contact with a ion-binding site in JP170, but not in Savinase. This knowledge opens for possibilities of adding or removing ion-binding sites to subtilases of the JP170 and BPN' like types.

A good example of the difference is the loop S232-K246 which has 15 residues compared to the corresponding BPN' type loop G211-T213 (in Savinase), which has only three residues. In the JP170 like subtilases, the loop folds back to the substrate binding site, especially the P' parts of the substrate binding site. The loop is situated close to the substrate as illustrated by the CI2 inhibitor bound in the 3D structure attached (Appendix 1).

The location of loop S232-K246 can be described in relation to the four specific residues as described above. The distance from the CA atom of residue W240 in the loop to the CA atoms of the active site residues are:

Residue	H68	D30	S254	M255
Distance, Å	11.45	18.51	13.06	11.94

As mentioned above, distances like these can vary ±0.80Å, preferably ±0.70Å, ±0.60Å, ±0.50Å, ±0.40Å, or most preferably ±0.30Å.

Furthermore, distances from the residues of JP170 loop S232-K246 to atoms of the CI2 inhibitor can be calculated. These distances are:
from CA atom of W240 to CA atom of R62 in CI2 is 7.49Å,
from CA atom of F239 to CA atom of R62 in CI2 is 8.39Å,
from CA atom of S238 to CA atom of R62 in CI2 is 8.42Å,
from CA atom of S237 to CA atom of R62 in CI2 is 9.44Å,
from CA atom of S238 to CA atom of E60 in CI2 is 9.42Å.

The distances from JP170 active site residue S254 to atoms of the CI2 inhibitor, as placed in the 3D coordinates of Appendix 1, are:
from CA atom of S254 to CA atom of E60 in CI2 is 5.25Å,
from CA atom of S254 to CA atom of R62 in CI2 is 11.55Å,
from CA atom of S254 to CA atom of T58 in CI2 is 7.06Å,
from CA atom of S254 to CA atom of M59 in CI2 is 4.71Å.
The distances can vary ±0.80Å, preferably ±0.70Å, ±0.60Å, ±0.50Å, ±0.40Å, or most preferably ±0.30Å.

A preferred JP170 like subtilase variant has a deletion in the region S232-K246, and the subsequent insertion of one or more residues to partly or completely remove the loop. Preferred variants comprises the deletion of L233-S245 + insertion of Asn, deletion of L233-D244 + insertion of Gly or deletion of S232-D244 + insertion of Gly.

Homology building of JP170 and BPN' subtilases

A model structure of a JP170 like subtilase or a BPN' like subtilase can be built using the Homology program or a comparable program, e.g., Modeller (both from Molecular Simulations, Inc., San Diego, CA). The principle is to align the amino acid sequence of a protein for which the 3D structure is known with the amino acid sequence of a protein for which a model 3D structure has to be constructed. The structurally conserved regions can then be built on the basis of consensus sequences. In areas lacking homology, loop structures can be inserted, or sequences can be deleted with subsequent bonding of the necessary residues using, e.g., the program Homology. Subsequent relaxing and optimization of the structure should be done using either Homology or another molecular simulation program, e.g., CHARMm from Molecular Simulations.

Methods for designing JP170 and BPN' subtilase variants

Comparisons of the molecular dynamics of different proteins can give a hint as to which domains are important or connected to certain properties pertained by each protein.

The present invention comprises a method of producing a variant of a parent JP170 like subtilase, the variant having at least one altered property as compared to the parent JP170 like subtilase, the method comprising:

a) modelling the parent JP170 subtilase on the three-dimensional structure of a JP170 subtilase to produce a three-dimensional structure of the parent JP170 subtilase;

b) identifying on the basis of the comparison in step a) at least one structural part of the parent JP170 subtilase, wherein an alteration in said structural part is predicted to result in an altered property;

c) modifying the nucleic acid sequence encoding the parent JP170 subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;

d) expressing the modified nucleic acid sequence in a host cell to produce the variant JP170 subtilase;

e) isolating the produced subtilase;

f) purifying the isolated subtilase and
g) recovering the purified subtilase.

Further the present invention comprises a method of producing a variant of a parent Subtilisin family subtilase, such as a BPN' like subtilase, the variant having at least one altered property as compared to the parent Subtilisin family subtilase, the method comprising:

a) modelling the parent Subtilisin family subtilase on the three-dimensional structure of a Subtilisin family subtilase to produce a three-dimensional structure of the parent Subtilisin family subtilase;
b) comparing the three-dimensional structure obtained in step a) to the three-dimensional structure of a JP170 like subtilase;
c) identifying on the basis of the comparison in step b) at least one structural part of the parent Subtilisin family subtilase, wherein an alteration in said structural part is predicted to result in an altered property;
d) modifying the nucleic acid sequence encoding the parent Subtilisin family subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;
e) expressing the modified nucleic acid sequence in a host cell to produce the variant Subtilisin family subtilase,
f) isolating the produced subtilase,
g) purifying the isolated subtilase and
h) recovering the purified subtilase.

Further the present invention comprises a method of producing a variant of a parent JP170 like subtilase, the variant having at least one altered property as compared to the parent JP170 like subtilase, the method comprising:

a) modelling the parent JP170 like subtilase on the three-dimensional structure of a JP170 like subtilase to produce a three-dimensional structure of the parent JP170 like subtilase;
b) comparing the three-dimensional structure obtained in step a) to the three-dimensional structure of a Subtilisin family subtilase;
c) identifying on the basis of the comparison in step b) at least one structural part of the parent JP170 like subtilase, wherein an alteration in said structural part is predicted to result in an altered property;

d) modifying the nucleic acid sequence encoding the parent JP170 like subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;

e) expressing the modified nucleic acid sequence in a host cell to produce the variant JP170 like subtilase;

f) isolating the produced subtilase;

g) purifying the isolated subtilase and

h) recovering the purified subtilase.

Stability - alteration of ion-binding sites

As described above the JP170 subtilases has three new ion-binding sites not present in the BPN' subtilisin structures but lacks the Strong and Weak ion-binding site of the BPN' subtilases. Stability of the ion-binding site is of crucial importance for the functionality of the enzyme. Therefore alterations of the ion-binding sites are likely to result in alterations of the stability of the enzyme.

Improved stability

Stabilisation of a JP170 subtilase may possibly be obtained by alterations in the positions close to the ion-binding sites. Thus a preferred variant of the present invention has a modification in one or more of the positions located at a distance of 10Å to the ion-binding sites of JP170 (SEQ ID NO:1). The positions are:

Site 1:	183-189	(i.e. positions 183, 184, 185, 186, 187, 188, 189),
	191-204	(i.e. positions 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204),
	224-225;	
Site 2:	378-393	(i.e. positions 378, 379, 380, 381, 382, 383, 384, 385, 386, 387, 388, 389, 390, 391, 392, 393);
Site 3:	348, 350, 352,	
	363-370	(i.e. positions 363, 364, 365, 366, 367, 368, 369, 370),
	380-383	(i.e. positions 380, 381, 382, 383),
	391-400	(i.e. positions 391, 392, 393, 394, 395, 396, 397, 398, 399, 400),

414-420 (i.e. positions 414, 415, 416, 417, 418, 419, 420).

In detergent compositions calcium chelaters contribute to removal of calcium from the subtilases with subsequent inactivation of the enzyme as the result. To decrease the inactivation due to calcium removal of e.g. calcium chelaters variants with improved calcium stability was constructed.

Preferred variants stabilised in ion-binding site 1 are S193Q,Y; H200D,N and H200D,N+D196N.

Preferred variants stabilised in ion-binding site 2 are N390D and N391D, and preferred variants stabilised in ion-binding site 3 are G394N,Q,F,Y,S and W392S,N,Q.

Alteration of thermostability

A variant with improved stability (typically increased thermostability) may be obtained by substitution with proline, introduction of a disulfide bond, altering a hydrogen bond contact, altering charge distribution, introduction of a salt bridge, filling in an internal structural cavity with one or more amino acids with bulkier side groups (in e.g. regions which are structurally mobile), substitution of histidine residues with other amino acids, removal of a deamidation sites, or by helix capping.

Regions with increased mobility:

The following regions of JP170 have an increased mobility in the crystal structure of the enzyme, and it is presently believed that these regions can be responsible for stability or activity of JP170. Especially thermostabilisation may possibly be obtained by altering the highly mobile regions. Improvements of the enzyme can be obtained by mutation in the below regions and positions. Introducing e.g. larger residues or residues having more atoms in the side chain could increase the stability, or, e.g., introduction of residues having fewer atoms in the side chain could be important for the mobility and thus the activity profile of the enzyme.

Two methods are used extract the highly mobile regions from a 3D structure. One is a molecular dynamics calculation of the isotropic fluctuations, and the other is an analysis of the B-factors. The B-factors are listed in the PDB file and give a value to the uncertainty of determination of the location of the various atoms of the structure. The uncertainty relates to the mobility of the atoms in the molecules in the crystal lattice. This mobility reflects the thermal motion of the atoms and thus indicates possible sites for thermostabilisation of the enzyme.

Thus, by analysing the B-factors taken from the coordinate file in Appendix 1, (see "in X-Ray Structure Determination, Stout, G.K. and Jensen, L.H., John Wiley & Sons, Inc. NY, 1989") the following mobile regions in the JP170 structure were revealed:

13-18 (i.e. positions 13, 14, 15, 16, 17, 18),
37-43 (i.e. positions 37, 38, 39, 40, 41, 42, 43),
47-50 (i.e. positions 47, 48, 49, 50),
57-59 (i.e. positions 57, 58, 59),
96-103 (i.e. positions 96, 97, 98, 99, 100, 101, 102, 103),
131-134 (i.e. positions 131, 132, 133, 134),
152-153
162-166 (i.e. positions 162, 163, 164, 165, 166),
188-195 (i.e. positions 188, 189, 190, 191, 192, 193, 194, 195),
210
234-246 (i.e. positions 234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246),
372-378 (i.e. positions 372, 373, 374, 375, 376, 377, 378),
387-392 (i.e. positions 387, 388, 389, 390, 391, 392),
406-407
419.

Molecular dynamics simulation at 300K and 400K of JP170 reveals the following highly mobile regions:

37-42 (i.e. positions 37, 38, 39, 40, 41, 42),
57-60 (i.e. positions 57, 58, 59, 60),
66-67,
98-103 (i.e. positions 98, 99, 100, 101, 102, 103),
107-111 (i.e. positions 107, 108, 109, 110, 111),
188-193 (i.e. positions 188, 189, 190, 191, 192, 193),
236-240 (i.e. positions 236, 237, 238, 239, 240),
326-332 (i.e. positions 326, 327, 328, 329, 330, 331, 332),
337-342 (i.e. positions 337, 338, 339, 340, 341, 342),
355-360 (i.e. positions 355, 356, 357, 358, 359, 360),
372-377 (i.e. positions 372, 373, 374, 375, 376, 377),

384-388 (i.e. positions 384, 385, 386, 387, 388),
404-411 (i.e. positions 404, 405, 406, 407, 408, 409, 410, 411).

Thus, a preferred JP170 subtilase variant of the present invention has been modified in one or more of the above mentioned positions of SEQ ID NO:1. Further preferred variants comprises one or more alterations in the regions 57-60, 66-67, 107-111, 236-240, 326-332, 355-360, 372-377, 384-388, 404-411. Especially preferred is variant W240H,Y and variants modified in the region 355-360, such as variants comprising one or more of the modifications: G355A,S; S356T,N; T357N,Q,D,E,P; T358S; A359S,T,N,Q and S360T,N.

Variants modified in the region 355-360 may be produced in accordance with the method for random mutagenesis by use of the DOPE program as described herein. To obtain variants comprising 1-3 modifications in region 355-360 one may introduce the substitutions with the following frequencies:

wild-type	modified	
95%	5%	G355A,S
90%	10%	S356T,N
80%	20%	T357N,Q,D,E,P
90%	10%	T358S
80%	20%	A359S,T,N,Q
80%	20%	S360T,N.

Disulfide bonds:

A JP170 variant of the present invention with improved stability, e.g. thermostability, as compared to the parent JP170 subtilase may be obtained by introducing new inter-domain or intra-domain bonds, such as by establishing inter- or intra-domain disulfide bridges.
Thus a further aspect of the present invention relates to a method for producing a variant of a parent JP170 comprising the methods described in the paragraph "Methods of preparing JP170 like or BPN' like subtilase variants" herein.

According to the guidelines mentioned above the below mentioned amino acid residues identified in the amino acid sequence of SEQ ID NO:1 are considered as being suitable for cysteine replacement. With one or more of these substitutions with cysteine, disulfide bridges may possibly form in a variant of JP170. The substitutions are: G21C/A86C, V26C/A265C, G57C/G105C, G74C/A229C, Q111C/Y143C, G160C/S170C, A286C/V349C,

A27C/A122C, A45C/G78C, V72C/P258C, G78C/A229C, D98C/G104C, Q111C/Y147C, G135C/G167C, R142C/P354C, V144C/A178C, G182C/P217C, A183C/G223C, A195C/Y225C, F271C/P279C, A287C/A430C, A293C/S310C, E322C/S428C, S324C/A332C, S327C/P424C, D352C/N397C, G255C/T362C, G291C/S314C.

Preferred variants comprise one or more of the substitutions: G21C/A86C, V26C/A265C, G57C/G105C, G74C/A229C, Q111C/Y143C, G160C/S170C, A286C/V349C, A4C/P222C and A27C/V117C.

Similar residues suitable for cysteine replacement in subtilases homologous with JP170 can be elucidated by finding the homologous positions in the alignment of Figure 1. Concerning another JP170 like sequence the homologous positions suitable for cysteine replacement can be selected by aligning said JP170 like sequence with all of the sequences of Figure 1 using the GAP analysis method as described above. The suitable residues can then be selected in accordance with the homologous positions in the most homologous of SEQ ID's NO:1, 2 and 3 which are the sequences of the subtilases aligned in Figure 1.

Surface charge distribution

A variant with improved stability (typically improved thermostability) as compared to the parent subtilase may be obtained by changing the surface charge distribution of the subtilase. For example, when the pH is lowered to about 5 or below histidine residues typically become positively charged and, consequently, unfavorable electrostatic interactions on the protein surface may occur. By engineering the surface charge of the subtilase one may avoid such unfavorable electrostatic interactions that in turn lead to a higher stability of the subtilase.

Therefore, a further aspect of the present invention relates to method for constructing a variant of a parent subtilase, the method comprising:

a) identifying, on the surface of the parent subtilase, preferably a JP170 like or a BPN' like subtilase, at least one amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His;

b) substituting, on the surface of the parent subtilase, at least one amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His with an uncharged amino acid residue;

c) optionally repeating steps a) and b) recursively;

d) optionally, making alterations each of which is an insertion, a deletion or a substitution of an amino acid residue at one or more positions other than b);
e) preparing the variant resulting from steps a) - d);
f) testing the stability of said variant; and
g) optionally repeating steps a) - f) recursively; and
h) selecting a subtilase variant having increased stability as compared to the parent subtilase.

As will be understood by the skilled person it may also, in some cases, be advantageous to substitute an uncharged amino acid residue with an amino acid residue bearing a charge or, alternatively, it may in some cases be advantageous to substitute an amino acid residue bearing a charge with an amino acid residue bearing a charge of opposite sign. Thus, the above-mentioned method may easily be employed by the skilled person also for these purposes. In the case of substituting an uncharged amino acid residue with an amino acid residue bearing a charge the above-mentioned method may be employed the only difference being steps a) and b) which will then read:

a) identifying, on the surface of the parent subtilase, at least one uncharged amino acid residue;
b) substituting, on the surface of the parent subtilase, at least one uncharged amino acid residue with a charged amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His.

Also in the case of changing the sign of an amino acid residue present on the surface of the subtilase the above method may be employed. Again, compared to the above method, the only difference being steps a) and b) which, in this case, read:

a) identifying, on the surface of the parent subtilase, at least one charged amino acid residue selected from the group consisting of Asp, Glu, Arg, Lys and His;
b) substituting, on the surface of the parent subtilase, at least one charged amino acid residue identified in step a) with an amino acid residue having an opposite charge.

Thus, Asp may be substituted with Arg, Lys or His; Glu may be substituted with Arg, Lys or His; Arg may be substituted with Asp or Glu; Lys may be substituted with Asp or Glu; and His may be substituted with Asp or Glu.

In order to determine the amino acid residues of a subtilase, which are present on the surface of the enzyme, the surface accessible area are measured using the DSSP program (Kabsch and Sander, *Biopolymers* (1983), 22, 2577-2637). All residues having a surface accessibilty higher than 0 is regarded a surface residue.

Amino acid residues found on the surface of JP170 using the above method are N76, N316, L381, K246, K9, K313 and K83. We consider the substitutions N79D, N316D and L381D of particular interest for stabilisation by introduction of salt bridges, whereas the substitutions K246R, K9R, K313R and K83R are of particular interest for the stabilisation at high pH.

Similar substitutions may be introduced in equivalent positions of other JP170 like subtilases.

Substitution with proline residues

Improved thermostability of a subtilase can be obtained by subjecting the subtilase in question to analysis for secondary structure, identifying residues in the subtilase having dihedral angles ϕ (phi) and ψ (psi) confined to the intervals [$-90° < \phi < -40°$ and $-180° < \psi < 180°$], preferably the intervals [$-90° < \phi < -40°$ and $120° < \psi < 180°$] or [$-90° < \phi < -40°$ and $-50° < \psi < 10°$] and excluding residues located in regions in which the subtilase is characterized by possessing α-helical or β-sheet structure.

After the dihedral angles ϕ (phi) and ψ (psi) for the amino acids have been calculated, based on the atomic structure in the crystalline subtilases, it is possible to select position(s) which has/have dihedral phi and psi angles favorable for substitution with a proline residue. The aliphatic side chain of proline residues is bonded covalently to the nitrogen atom of the peptide group. The resulting cyclic five-membered ring consequently imposes a rigid constraint on the rotation about the N-C_α bond of the peptide backbone and simultaneously prevents the formation of hydrogen bonding to the backbone N-atom. For these structural reasons, proline residues are generally not compatible with α-helical and β-sheet secondary conformations.

If a proline residue is not already at the identified position(s), the naturally occurring amino acid residue is substituted with a proline residue, preferably by site directed mutagenesis applied on a gene encoding the subtilase in question.

In the group of JP170 like subtilases proline residues can advantageously be introduced at positions 22, 44, 110, 139, 140, 166, 198, 201, 203, 231, 282, 356, 357 and 378. Accordingly, a preferred JP170 variant has one or more of the substitutions: Q22P, E44P, L110P,

T139P, D140P, S166P I198P, V201P, Q203P, S231P, S282P, S356P, T357P and K378P. Especially preferred are variants comprising one or more of: E44P, Q203P and S356P.

Improved activity of JP170 subtilases

As mentioned the JP170 subtilases differ greatly from the BPN' like subtilases in having a long apparently non-catalytic C-terminal. A possible truncation of JP170 is the removal of approx. 115 residues including two ion-binding sites, which can be obtained by deletion of or within the region 311-433, which is non-catalytic C-terminal. Preferred deletions are of the regions 317-433 or 315-433. Preferably the new C-terminal will be within the region of 311-325. Further, the deletion can be optimised with additional substitutions, such as one or more of L283N,Q; A290S,N and W306H,Y,K.

Preferred truncations comprise:

a) deletion of region 317-433 and the substitutions L283N + A290S + W306H,

b) deletion of region 315-433 and the substitutions L283N + A290S + W306H.

Substrate binding site

The substrate binding site is identified by the residues in contact with a substrate model, such as the CI2 inhibitor. The 3D structure coordinates of the JP170 subtilase with CI2 bound in the active site can be found in Appendix 1. Without being limited to any theory, it is presently believed that binding between a substrate and an enzyme is supported by favorable interactions found within a sphere 10 Å from the substrate molecule. Examples of such favorable bonds are hydrogen bonds, strong electrostatic interaction and/or hydrophobic interactions.

The following residues of the JP170 subtilase (SEQ ID NO:1), are within a distance of 10Å from the CI2 inhibitor which is bound to the substrate binding site. These residues are thus believed to be involved in interactions with said substrate:

29-32, (i.e. residues 29, 30, 31, 32)
64-72, (i.e. residues 64, 65, 66, 67, 68, 69, 70, 71, 72)
93,
96-98, (i.e. residues 96, 97, 98)
100-110, (i.e. residues 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110)
113-114,
127-136, (i.e. residues 127, 128, 129, 130, 131, 132, 133, 134, 135, 136)
138-141, (i.e. residues 138, 139, 140, 141)
144, 157, 174,

180-183, (i.e. residues 180, 181, 182, 183)
191, 193-194,
202-207, (i.e. residues 202, 203, 204, 205, 206, 207)
211,
223-226, (i.e. residues 223, 224, 225, 226)
234-241, (i.e. residues 234, 235, 236, 237, 238, 239, 240, 241)
249-258 (i.e. residues 249, 250, 251, 252, 253, 254, 255, 256, 257, 258).

In an embodyment of the present invention a variant comprises a modification in one or more of the above mentioned positions. A preferred variants is W129L.

JP170 with extra ion-binding site

The Strong ion-binding site from the BPN' subtilases can be transplanted into JP170 (or other subtilases in JP170 subgroup) by deletion of N79-N82 and subsequent insertion of LNNSIGV, followed by the substitution A45D,N and optionally the substitutions E44P,T and/or R47Q.

Removal of ion-binding site in JP170

By removing an ion-binding site it is possible to decrease the enzymes dependency of calcium in the media. The ion-binding sites in JP170 (or others from JP170 group) can be removed with guidance from the three-dimensional structure of BPN' and Savinase (or others in BPN' group), and of TY145 like subtilases.

Removal of ion-binding site 1 can be done by deletion of N186-N199 and subsequent insertion of at least three amino acid residues, preferably the sequence SSN. Preferably, but not mandatory one or both of the substitutions I7Q and V3Y is further added.

The ion-binding site 1 can be removed from a wild-type JP170 subtilase or a JP170 subtilase truncated as described above.

Subtilases free of ion-binding sites

With guidance from the three-dimensional structure of JP170 like subtilases and of TY145 like subtilases, the Strong and Weak ion-binding sites in BPN' like subtilases can be removed. Likewise, as described above, with guidance from the three-dimensional structure of BPN' and Savinase (or others in BPN' group), and of TY145 like subtilases, all three ion-binding sites can be removed from the wild-type JP170 subtilase or from JP170 like subti-

lases. The same approach can be used to remove the ion-binding sites from TY145 like subtilases.

Exemplified in Savinase, the removal can be done by altering the loops A194-L196 and L75-L82 either by a) insertion or deletion of a number of amino acid residues in the loops or b) by deletion of the entire loop or part of the loop and subsequent insertion of a number of residues from a corresponding loop of a JP170 or TY145 like subtilase.

Preferably the ion-binding sites of Savinase can be removed by either

i) deletion of or in the region A194-L196 (BPN' numbers) and insertion of three or more residues chosen from JP170 positions P209-P217 and
deletion of or in the region L75-L82 (BPN' numbers) and insertion of at least one residue chosen from TY145 positions H83-Y92 or

ii) deletion of or in the region A194-L196 (BPN' numbers) and insertion of three or more residues chosen from JP170 positions P209-P217 and
deletion of or in the region L75-L82 (BPN' numbers) and insertion of at least one residues chosen from JP170 positions N79-K83.

Combined modifications

The present invention also encompasses any of the above mentioned subtilase variants in combination with any other modification to the amino acid sequence thereof. Especially combinations with other modifications known in the art to provide improved properties to the enzyme are envisaged.

Such combinations comprise the positions: 222 (improves oxidation stability), 218 (improves thermal stability), substitutions in the Ca^{2+}-binding sites stabilizing the enzyme, *e.g.* position 76, and many other apparent from the prior art.

In further embodiments a subtilase variant described herein may advantageously be combined with one or more modification(s) in any of the positions:

27, 36, 56, 76, 87, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 120, 123, 159, 167, 170, 206, 218, 222, 224, 232, 235, 236, 245, 248, 252 and 274 (BPN' numbering).

Specifically, the following BLSAVI, BLSUBL, BSKSMK, and BAALKP modifications are considered appropriate for combination:

K27R, *36D, S56P, N76D, S87N, G97N, S101G, S103A, V104A, V104I, V104N, V104Y, H120D, N123S, G159D, Y167, R170, Q206E, N218S, M222S, M222A, T224S, A232V, K235L, Q236H, Q245R, N248D, N252K and T274A.

Furthermore variants comprising any of the modifications S101G+V104N, S87N+S101G+V104N, K27R+V104Y+N123S+T274A, N76D+S103A+V104I or N76D+V104A, or other combinations of the modifications K27R, N76D, S101G, S103A, V104N, V104Y, V104I, V104A, N123S, G159D, A232V, Q236H, Q245R, N248D, N252K, T274A in combination with any one or more of the modification(s) mentioned above exhibit improved properties.

A particular interesting variant is a variant, which, in addition to modifications according to the invention, contains the following substitutions:

S101G+S103A+V104I+G159D+A232V+Q236H+Q245R+N248D+N252K.

Moreover, subtilase variants of the main aspect(s) of the invention are preferably combined with one or more modification(s) in any of the positions 129, 131 and 194, preferably as 129K, 131H and 194P modifications, and most preferably as P129K, P131H and A194P modifications. Any of those modification(s) are expected to provide a higher expression level of the subtilase variant in the production thereof.

Stabilization by modification of Asn-Gly pairs

It is known that at alkaline pH, the side chain of Asn may interact with the NH group of a sequential neighbouring amino acid to form an isoAsp residue where the backbone goes through the Asp side chain. This will leave the backbone more vulnerable to proteolysis. The deamidation is much more likely to occur if the residue that follows is a Gly. Changing the Asn in front of the Gly or the Gly will prevent this from happening and thus improve the stability, especially as concerns thermo- and storage stability.

The invention consequently further relates to a subtilase, in which either or both residues of any of the Asn-Gly sequence appearing in the amino acid sequence of the parent RP-II protease is/are deleted or substituted with a residue of a different amino acid.

The Asn and/or Gly residue may, for instance, be substituted with a residue of an amino acid selected from the group consisting of A, Q, S, P, T and Y.

Modification of Tyrosine residues

In relation to wash performance it has been found that the modification of certain tyrosine residues to phenylalanine provides an improved wash performance. Without being bound by any specific theory, it is believed that titration of these Tyr residues in the alkaline wash liquor has negative effects that are alleviated by replacing the Tyr residues with other residues, especially Phe or Trp, particularly Phe.

Methods of preparing JP170 like or BPN' like subtilase variants

The subtilase variants, i.e. the JP170 and BPN' variants of the present invention may be produced by any known method within the art and the present invention also relates to nucleic acid encoding a subtilase variant of the present invention, a DNA construct comprising said nucleic acid and a host cell comprising said nucleic acid sequence.

In general natural occurring proteins may be produced by culturing the organism expressing the protein and subsequently purifying the protein or it may be produced by cloning a nucleic acid, e.g. genomic DNA or cDNA, encoding the protein into an expression vector, introducing said expression vector into a host cell, culturing the host cell and purifying the expressed protein.

Typically protein variants may be produced by site-directed mutagenesis of a parent protein, introduction into expression vector, host cell etc. The parent protein may be cloned from a strain producing the polypeptide or from an expression library, i.e. it may be isolated from genomic DNA or prepared from cDNA, or a combination thereof.

In general standard procedures for cloning of genes and/or introducing mutations (random and/or site directed) into said genes may be used in order to obtain a parent subtilase, or subtilase or subtilase variant of the invention. For further description of suitable techniques reference is made to Molecular cloning: A laboratory manual (Sambrook et al. (1989), Cold Spring Harbor lab., Cold Spring Harbor, NY; Ausubel, F. M. et al. (eds.)); Current protocols in Molecular Biology (John Wiley and Sons, 1995; Harwood, C. R., and Cutting, S. M. (eds.)); Molecular Biological Methods for Bacillus (John Wiley and Sons, 1990); DNA Cloning: A Practical Approach, Volumes I and II (D.N. Glover ed. 1985); Oligonucleotide Synthesis (M.J. Gait ed. 1984); Nucleic Acid Hybridization (B.D. Hames & S.J. Higgins eds (1985)); Transcription And Translation (B.D. Hames & S.J. Higgins, eds. (1984)); Animal Cell Culture (R.I. Freshney, ed. (1986)); Immobilized Cells And Enzymes (IRL Press, (1986)); A Practical Guide To Molecular Cloning (B. Perbal, (1984)) and WO 96/34946.

Further, variants could be constructed by:

Random Mutagenesis

Random mutagenesis is suitably performed either as localized or region-specific random mutagenesis in at least three parts of the gene translating to the amino acid sequence shown in question, or within the whole gene.

The random mutagenesis of a DNA sequence encoding a parent subtilase may be conveniently performed by use of any method known in the art.

In relation to the above, a further aspect of the present invention relates to a method for generating a variant of a parent subtilase, wherein the variant exhibits an altered property, such as increased thermostability, increased stability at low pH and at low calcium concentration, relative to the parent subtilase, the method comprising:

(a) subjecting a DNA sequence encoding the parent subtilase to random mutagenesis,

(b) expressing the mutated DNA sequence obtained in step (a) in a host cell, and

(c) screening for host cells expressing a subtilase variant which has an altered property relative to the parent subtilase.

Step (a) of the above method of the invention is preferably performed using doped primers. For instance, the random mutagenesis may be performed by use of a suitable physical or chemical mutagenizing agent, by use of a suitable oligonucleotide, or by subjecting the DNA sequence to PCR generated mutagenesis. Furthermore, the random mutagenesis may be performed by use of any combination of these mutagenizing agents. The mutagenizing agent may, e.g., be one which induces transitions, transversions, inversions, scrambling, deletions, and/or insertions.

Examples of a physical or chemical mutagenizing agent suitable for the present purpose include ultraviolet (UV) irradiation, hydroxylamine, N-methyl-N'-nitro-N-nitrosoguanidine (MNNG), O-methyl hydroxylamine, nitrous acid, ethyl methane sulphonate (EMS), sodium bisulphite, formic acid, and nucleotide analogues. When such agents are used, the mutagenesis is typically performed by incubating the DNA sequence encoding the parent enzyme to be mutagenized in the presence of the mutagenizing agent of choice under suitable conditions for the mutagenesis to take place, and selecting for mutated DNA having the desired properties.

When the mutagenesis is performed by the use of an oligonucleotide, the oligonucleotide may be doped or spiked with the three non-parent nucleotides during the synthesis of the oligonucleotide at the positions that are to be changed. The doping or spiking may be done so that codons for unwanted amino acids are avoided. The doped or spiked oligonucleotide

can be incorporated into the DNA encoding the subtilase enzyme by any published technique, using, e.g., PCR, LCR or any DNA polymerase and ligase as deemed appropriate.

Preferably, the doping is carried out using "constant random doping", in which the percentage of wild-type and modification in each position is predefined. Furthermore, the doping may be directed toward a preference for the introduction of certain nucleotides, and thereby a preference for the introduction of one or more specific amino acid residues. The doping may be made, e.g., so as to allow for the introduction of 90% wild type and 10% modifications in each position. An additional consideration in the choice of a doping scheme is based on genetic as well as protein-structural constraints. The doping scheme may be made by using the DOPE program which, *inter alia*, ensures that introduction of stop codons is avoided (L.J. Jensen et al. *Nucleic Acid Research*, 26, 697-702 (1998).

When PCR-generated mutagenesis is used, either a chemically treated or non-treated gene encoding a parent subtilase enzyme is subjected to PCR under conditions that increase the misincorporation of nucleotides (Deshler 1992; Leung et al., *Technique*, 1, 1989, pp. 11-15).

A mutator strain of *E. coli* (Fowler et al., *Molec. Gen. Genet.*, 133, 1974, 179-191), *S. cerevisiae* or any other microbial organism may be used for the random mutagenesis of the DNA encoding the subtilase by, e.g., transforming a plasmid containing the parent enzyme into the mutator strain, growing the mutator strain with the plasmid and isolating the mutated plasmid from the mutator strain. The mutated plasmid may be subsequently transformed into the expression organism.

The DNA sequence to be mutagenized may conveniently be present in a genomic or cDNA library prepared from an organism expressing the parent subtilase. Alternatively, the DNA sequence may be present on a suitable vector such as a plasmid or a bacteriophage, which as such may be incubated with or otherwise exposed to the mutagenising agent. The DNA to be mutagenized may also be present in a host cell either by being integrated in the genome of said cell or by being present on a vector harbored in the cell. Finally, the DNA to be mutagenized may be in isolated form. It will be understood that the DNA sequence to be subjected to random mutagenesis is preferably a cDNA or a genomic DNA sequence.

In some cases it may be convenient to amplify the mutated DNA sequence prior to performing the expression step b) or the screening step c). Such amplification may be performed in accordance with methods known in the art, the presently preferred method being PCR-generated amplification using oligonucleotide primers prepared on the basis of the DNA or amino acid sequence of the parent enzyme.

Subsequent to the incubation with or exposure to the mutagenising agent, the mutated DNA is expressed by culturing a suitable host cell carrying the DNA sequence under conditions allowing expression to take place. The host cell used for this purpose may be one which has been transformed with the mutated DNA sequence, optionally present on a vector, or one which was carried the DNA sequence encoding the parent enzyme during the mutagenesis treatment. Examples of suitable host cells are the following: gram positive bacteria such as *Bacillus subtilis*, *Bacillus licheniformis*, *Bacillus lentus*, *Bacillus brevis*, *Bacillus stearothermophilus*, *Bacillus alkalophilus*, *Bacillus amyloliquefaciens*, *Bacillus coagulans*, *Bacillus circulans*, *Bacillus lautus*, *Bacillus megaterium*, *Bacillus thuringiensis*, *Streptomyces lividans* or *Streptomyces murinus*; and gram negative bacteria such as *E. coli*. The mutated DNA sequence may further comprise a DNA sequence encoding functions permitting expression of the mutated DNA sequence.

Localised random mutagenesis

The random mutagenesis may be advantageously localised to a part of the parent subtilase in question. This may, e.g., be advantageous when certain regions of the enzyme have been identified to be of particular importance for a given property of the enzyme, and when modified are expected to result in a variant having improved properties. Such regions may normally be identified when the tertiary structure of the parent enzyme has been elucidated and related to the function of the enzyme.

The localised or region-specific, random mutagenesis is conveniently performed by use of PCR generated mutagenesis techniques as described above or any other suitable technique known in the art. Alternatively, the DNA sequence encoding the part of the DNA sequence to be modified may be isolated, e.g., by insertion into a suitable vector, and said part may be subsequently subjected to mutagenesis by use of any of the mutagenesis methods discussed above.

General method for random mutagenesis by use of the DOPE program

The random mutagenesis may be carried out by the following steps:

1. Select regions of interest for modification in the parent enzyme
2. Decide on mutation sites and non-mutated sites in the selected region
3. Decide on which kind of mutations should be carried out, e.g. with respect to the desired stability and/or performance of the variant to be constructed
4. Select structurally reasonable mutations
5. Adjust the residues selected by step 3 with regard to step 4.

6. Analyse by use of a suitable dope algorithm the nucleotide distribution.
7. If necessary, adjust the wanted residues to genetic code realism, e.g. taking into account constraints resulting from the genetic code, e.g. in order to avoid introduction of stop codons; the skilled person will be aware that some codon combinations cannot be used in practice and will need to be adapted
8. Make primers
9. Perform random mutagenesis by use of the primers
10. Select resulting subtilase variants by screening for the desired improved properties.

Suitable dope algorithms for use in step 6 are well known in the art. One such algorithm is described by Tomandl, D. et al., 1997, Journal of Computer-Aided Molecular Design 11:29-38. Another algorithm is DOPE (Jensen, LJ, Andersen, KV, Svendsen, A, and Kretzschmar, T (1998) Nucleic Acids Research 26:697-702).

Expression vectors

A recombinant expression vector comprising a nucleic acid sequence encoding a subtilase variant of the invention may be any vector that may conveniently be subjected to recombinant DNA procedures and which may bring about the expression of the nucleic acid sequence.

The choice of vector will often depend on the host cell into which it is to be introduced. Examples of a suitable vector include a linear or closed circular plasmid or a virus. The vector may be an autonomously replicating vector, i.e., a vector which exists as an extra-chromosomal entity, the replication of which is independent of chromosomal replication, e.g., a plasmid, an extra-chromosomal element, a mini chromosome, or an artificial chromosome. The vector may contain any means for assuring self-replication. Examples of bacterial origins of replication are the origins of replication of plasmids pBR322, pUC19, pACYC177, pACYC184, pUB110, pE194, pTA1060, and pAMß1. Examples of origin of replications for use in a yeast host cell are the 2 micron origin of replication, the combination of CEN6 and ARS4, and the combination of CEN3 and ARS1. The origin of replication may be one having a mutation which makes it function as temperature-sensitive in the host cell (see, e.g., Ehrlich, 1978, Proceedings of the National Academy of Sciences USA 75:1433).

Alternatively, the vector may be one which, when introduced into the host cell, is integrated into the genome and replicated together with the chromosome(s) into which it has been integrated. Vectors which are integrated into the genome of the host cell may contain any

nucleic acid sequence enabling integration into the genome, in particular it may contain nucleic acid sequences facilitating integration into the genome by homologous or non-homologous recombination. The vector system may be a single vector, e.g. plasmid or virus, or two or more vectors, e.g. plasmids or virus', which together contain the total DNA to be introduced into the genome of the host cell, or a transposon.

The vector may in particular be an expression vector in which the DNA sequence encoding the subtilase variant of the invention is operably linked to additional segments or control sequences required for transcription of the DNA. The term, "operably linked" indicates that the segments are arranged so that they function in concert for their intended purposes, e.g. transcription initiates in a promoter and proceeds through the DNA sequence encoding the subtilase variant. Additional segments or control sequences include a promoter, a leader, a polyadenylation sequence, a propeptide sequence, a signal sequence and a transcription terminator. At a minimum the control sequences include a promoter and transcriptional and translational stop signals.

The promoter may be any DNA sequence that shows transcriptional activity in the host cell of choice and may be derived from genes encoding proteins either homologous or heterologous to the host cell.

Examples of suitable promoters for use in bacterial host cells include the promoter of the *Bacillus subtilis* levansucrase gene (sacB), the *Bacillus stearothermophilus* maltogenic amylase gene (amyM), the *Bacillus licheniformis* alpha-amylase gene (amyL), the *Bacillus amyloliquefaciens* alpha-amylase gene (amyQ), the *Bacillus subtilis* alkaline protease gene, or the *Bacillus pumilus* xylosidase gene, the *Bacillus amyloliquefaciens* BAN amylase gene, the *Bacillus licheniformis* penicillinase gene (penP), the *Bacillus subtilis* xylA and xylB genes, and the prokaryotic beta-lactamase gene (Villa-Kamaroff et al., 1978, Proceedings of the National Academy of Sciences USA 75:3727-3731). Other examples include the phage Lambda P_R or P_L promoters or the E. coli lac, trp or tac promoters or the Streptomyces coelicolor agarase gene (dagA). Further promoters are described in "Useful proteins from recombinant bacteria" in Scientific American, 1980, 242:74-94; and in Sambrook et al., 1989, supra.

Examples of suitable promoters for use in a filamentous fungal host cell are promoters obtained from the genes encoding *Aspergillus oryzae* TAKA amylase, *Rhizomucor miehei* aspartic proteinase, *Aspergillus niger* neutral alpha-amylase, *Aspergillus niger* acid stable alpha-amylase, *Aspergillus niger* or *Aspergillus awamori* glucoamylase (glaA), *Rhizomucor miehei* lipase, *Aspergillus oryzae* alkaline protease, *Aspergillus oryzae* triose phosphate isomerase, *Aspergillus nidulans* acetamidase, *Fusarium oxysporum* trypsin-like protease

(as described in U.S. Patent No. 4,288,627, which is incorporated herein by reference), and hybrids thereof. Particularly preferred promoters for use in filamentous fungal host cells are the TAKA amylase, NA2-tpi (a hybrid of the promoters from the genes encoding *Aspergillus niger* neutral (-amylase and *Aspergillus oryzae* triose phosphate isomerase), and glaA promoters. Further suitable promoters for use in filamentous fungus host cells are the ADH3 promoter (McKnight et al., The EMBO J. 4 (1985), 2093 - 2099) or the tpiA promoter. Examples of suitable promoters for use in yeast host cells include promoters from yeast glycolytic genes (Hitzeman et al., J. Biol. Chem. 255 (1980), 12073 - 12080; Alber and Kawasaki, J. Mol. Appl. Gen. 1 (1982), 419 - 434) or alcohol dehydrogenase genes (Young et al., in Genetic Engineering of Microorganisms for Chemicals (Hollaender et al, eds.), Plenum Press, New York, 1982), or the TPI1 (US 4,599,311) or ADH2-4c (Russell et al., Nature 304 (1983), 652 - 654) promoters.

Further useful promoters are obtained from the *Saccharomyces cerevisiae* enolase (ENO-1) gene, the *Saccharomyces cerevisiae* galactokinase gene (GAL1), the *Saccharomyces cerevisiae* alcohol dehydrogenase/glyceraldehyde-3-phosphate dehydrogenase genes (ADH2/GAP), and the *Saccharomyces cerevisiae* 3-phosphoglycerate kinase gene. Other useful promoters for yeast host cells are described by Romanos et al., 1992, Yeast 8:423-488. In a mammalian host cell, useful promoters include viral promoters such as those from Simian Virus 40 (SV40), Rous sarcoma virus (RSV), adenovirus, and bovine papilloma virus (BPV).

Examples of suitable promoters for use in mammalian cells are the SV40 promoter (Subramani et al., Mol. Cell Biol. 1 (1981), 854 -864), the MT-1 (metallothionein gene) promoter (Palmiter et al., Science 222 (1983), 809 - 814) or the adenovirus 2 major late promoter.

An example of a suitable promoter for use in insect cells is the polyhedrin promoter (US 4,745,051; Vasuvedan et al., FEBS Lett. 311, (1992) 7 - 11), the P10 promoter (J.M. Vlak et al., J. Gen. Virology 69, 1988, pp. 765-776), the Autographa californica polyhedrosis virus basic protein promoter (EP 397 485), the baculovirus immediate early gene 1 promoter (US 5,155,037; US 5,162,222), or the baculovirus 39K delayed-early gene promoter (US 5,155,037; US 5,162,222).

The DNA sequence encoding a subtilase variant of the invention may also, if necessary, be operably connected to a suitable terminator.

The recombinant vector of the invention may further comprise a DNA sequence enabling the vector to replicate in the host cell in question.

The vector may also comprise a selectable marker, e.g. a gene the product of which complements a defect in the host cell, or a gene encoding resistance to e.g. antibiotics like ampicillin, kanamycin, chloramphenicol, erythromycin, tetracycline, spectinomycine, neomycin, hygromycin, methotrexate, or resistance to heavy metals, virus or herbicides, or which provides for prototrophy or auxotrophs. Examples of bacterial selectable markers are the dal genes from *Bacillus subtilis* or *Bacillus licheniformis*, resistance. A frequently used mammalian marker is the dihydrofolate reductase gene (DHFR). Suitable markers for yeast host cells are ADE2, HIS3, LEU2, LYS2, MET3, TRP1, and URA3. A selectable marker for use in a filamentous fungal host cell may be selected from the group including, but not limited to, amdS (acetamidase), argB (ornithine carbamoyltransferase), bar (phosphinothricin acetyltransferase), hygB (hygromycin phosphotransferase), niaD (nitrate reductase), pyrG (orotidine-5'-phosphate decarboxylase), sC (sulfate adenyltransferase), trpC (anthranilate synthase), and glufosinate resistance markers, as well as equivalents from other species. Particularly, for use in an *Aspergillus* cell are the amdS and pyrG markers of *Aspergillus nidulans* or *Aspergillus oryzae* and the bar marker of *Streptomyces hygroscopicus*. Furthermore, selection may be accomplished by co-transformation, e.g., as described in WO 91/17243, where the selectable marker is on a separate vector.

To direct a subtilase variant of the present invention into the secretory pathway of the host cells, a secretory signal sequence (also known as a leader sequence, prepro sequence or pre sequence) may be provided in the recombinant vector. The secretory signal sequence is joined to the DNA sequence encoding the enzyme in the correct reading frame. Secretory signal sequences are commonly positioned 5' to the DNA sequence encoding the enzyme. The secretory signal sequence may be that normally associated with the enzyme or may be from a gene encoding another secreted protein.

The procedures used to ligate the DNA sequences coding for the present enzyme, the promoter and optionally the terminator and/or secretory signal sequence, respectively, or to assemble these sequences by suitable PCR amplification schemes, and to insert them into suitable vectors containing the information necessary for replication or integration, are well known to persons skilled in the art (cf., for instance, Sambrook et al.).

More than one copy of a nucleic acid sequence encoding an enzyme of the present invention may be inserted into the host cell to amplify expression of the nucleic acid sequence. Stable amplification of the nucleic acid sequence can be obtained by integrating at least one additional copy of the sequence into the host cell genome using methods well known in the art and selecting for transformants.

The nucleic acid constructs of the present invention may also comprise one or more nucleic acid sequences which encode one or more factors that are advantageous in the expression of the polypeptide, e.g., an activator (e.g., a trans-acting factor), a chaperone, and a processing protease. Any factor that is functional in the host cell of choice may be used in the present invention. The nucleic acids encoding one or more of these factors are not necessarily in tandem with the nucleic acid sequence encoding the polypeptide.

Host cells

The DNA sequence encoding a subtilase variant of the present invention may be either homologous or heterologous to the host cell into which it is introduced. If homologous to the host cell, i.e. produced by the host cell in nature, it will typically be operably connected to another promoter sequence or, if applicable, another secretory signal sequence and/or terminator sequence than in its natural environment. The term "homologous" is intended to include a DNA sequence encoding an enzyme native to the host organism in question. The term "heterologous" is intended to include a DNA sequence not expressed by the host cell in nature. Thus, the DNA sequence may be from another organism, or it may be a synthetic sequence.

The host cell into which the DNA construct or the recombinant vector of the invention is introduced may be any cell that is capable of producing the present subtilase variants, such as prokaryotes, e.g. bacteria or eukaryotes, such as fungal cells, e.g. yeasts or filamentous fungi, insect cells, plant cells or mammalian cells.

Examples of bacterial host cells which, on cultivation, are capable of producing the subtilase variants of the invention are gram-positive bacteria such as strains of *Bacillus*, e.g. strains of *B. subtilis*, *B. licheniformis*, *B. lentus*, *B. brevis*, *B. stearothermophilus*, *B. alkalophilus*, *B. amyloliquefaciens*, *B. coagulans*, *B. circulans*, *B. lautus*, *B. megaterium* or *B. thuringiensis*, or strains of *Streptomyces*, such as *S. lividans* or *S. murinus*, or gram-negative bacteria such as *Escherichia coli* or *Pseudomonas sp.*

The transformation of the bacteria may be effected by protoplast transformation, electroporation, conjugation, or by using competent cells in a manner known per se (cf. Sambrook et al., supra).

When expressing the subtilase variant in bacteria such as *E. coli*, the enzyme may be retained in the cytoplasm, typically as insoluble granules (known as inclusion bodies), or it may be directed to the periplasmic space by a bacterial secretion sequence. In the former case, the cells are lysed and the granules are recovered and denatured after which the enzyme is refolded by diluting the denaturing agent. In the latter case, the enzyme may be

recovered from the periplasmic space by disrupting the cells, e.g. by sonication or osmotic shock, to release the contents of the periplasmic space and recovering the enzyme.

When expressing the subtilase variant in gram-positive bacteria such as *Bacillus* or *Streptomyces* strains, the enzyme may be retained in the cytoplasm, or it may be directed to the extracellular medium by a bacterial secretion sequence. In the latter case, the enzyme may be recovered from the medium as described below.

Examples of host yeast cells include cells of a species of *Candida*, *Kluyveromyces*, *Saccharomyces*, *Schizosaccharomyces*, *Pichia*, *Hansehula*, or *Yarrowia*. In a particular embodiment, the yeast host cell is a *Saccharomyces carlsbergensis*, *Saccharomyces cerevisiae*, *Saccharomyces diastaticus*, *Saccharomyces douglasii*, *Saccharomyces kluyveri*, *Saccharomyces norbensis* or *Saccharomyces oviformis* cell. Other useful yeast host cells are a *Kluyveromyces lactis*, *Kluyveromyces fragilis*, *Hansehula polymorpha*, *Pichia pastoris*, *Yarrowia lipolytica*, *Schizosaccharomyces pombe*, *Ustilgo maylis*, *Candida maltose*, *Pichia guillermondii* and *Pichia methanolio* cell (cf. Gleeson et al., J. Gen. Microbiol. 132, 1986, pp. 3459-3465; US 4,882,279 and US 4,879,231). Since the classification of yeast may change in the future, for the purposes of this invention, yeast shall be defined as described in Biology and Activities of Yeast (Skinner, F.A., Passmore, S.M., and Davenport, R.R., eds, Soc. App. Bacteriol. Symposium Series No. 9, 1980. The biology of yeast and manipulation of yeast genetics are well known in the art (see, e.g., Biochemistry and Genetics of Yeast, Bacil, M., Horecker, B.J., and Stopani, A.O.M., editors, 2nd edition, 1987; The Yeasts, Rose, A.H., and Harrison, J.S., editors, 2nd edition, 1987; and The Molecular Biology of the Yeast Saccharomyces, Strathern et al., editors, 1981). Yeast may be transformed using the procedures described by Becker and Guarente, In Abelson, J.N. and Simon, M.I., editors, Guide to Yeast Genetics and Molecular Biology, Methods in Enzymology, Volume 194, pp 182-187, Academic Press, Inc., New York; Ito et al., 1983, Journal of Bacteriology 153:163; and Hinnen et al., 1978, Proceedings of the National Academy of Sciences USA 75:1920.

Examples of filamentous fungal cells include filamentous forms of the subdivision Eumycota and Oomycota (as defined by Hawksworth et al., 1995, supra), in particular it may of the a cell of a species of *Acremonium*, such as *A. chrysogenum*, *Aspergillus*, such as *A. awamori*, *A. foetidus*, *A. japonicus*, *A. niger*, *A. nidulans* or *A. oryzae*, *Fusarium*, such as *F. bactridioides*, *F. cerealis*, *F. crookwellense*, *F. culmorum*, *F. graminearum*, *F. graminum*, *F. heterosporum*, *F. negundi*, *F. reticulatum*, *F. roseum*, *F. sambucinum*, *F. sarcochroum*, *F. sulphureum*, *F. trichothecioides* or *F. oxysporum*, *Humicola*, such as *H. insolens* or *H. lanuginose*, *Mucor*, such as *M. miehei*, *Myceliophthora*, such as *M. thermophilum*, *Neuro-*

spora, such as *N. crassa*, *Penicillium*, such as *P. purpurogenum*, *Thielavia*, such as *T. terrestris*, *Tolypocladium*, or *Trichoderma*, such as *T. harzianum*, *T. koningii*, *T. longibrachiatum*, *T. reesei* or *T. viride*, or a teleomorph or synonym thereof. The use of *Aspergillus spp.* for the expression of proteins is described in, e.g., EP 272 277, EP 230 023.

Examples of insect cells include a *Lepidoptera* cell line, such as *Spodoptera frugiperda* cells or *Trichoplusia ni* cells (cf. US 5,077,214). Culture conditions may suitably be as described in WO 89/01029 or WO 89/01028.Transformation of insect cells and production of heterologous polypeptides therein may be performed as described in US 4,745,051; US 4,775, 624; US 4,879,236; US 5,155,037; US 5,162,222; EP 397,485).

Examples of mammalian cells include Chinese hamster ovary (CHO) cells, HeLa cells, baby hamster kidney (BHK) cells, COS cells, or any number of other immortalized cell lines available, e.g., from the American Type Culture Collection. Methods of transfecting mammalian cells and expressing DNA sequences introduced in the cells are described in e.g. Kaufman and Sharp, J. Mol. Biol. 159 (1982), 601 - 621; Southern and Berg, J. Mol. Appl. Genet. 1 (1982), 327 - 341; Loyter et al., Proc. Natl. Acad. Sci. USA 79 (1982), 422 - 426; Wigler et al., Cell 14 (1978), 725; Corsaro and Pearson, Somatic Cell Genetics 7 (1981), 603, Ausubel et al., Current Protocols in Molecular Biology, John Wiley and Sons, Inc., N.Y., 1987, Hawley-Nelson et al., Focus 15 (1993), 73; Ciccarone et al., Focus 15 (1993), 80; Graham and van der Eb, Virology 52 (1973), 456; and Neumann et al., EMBO J. 1 (1982), 841 - 845. Mammalian cells may be transfected by direct uptake using the calcium phosphate precipitation method of Graham and Van der Eb (1978, Virology 52:546).

Methods for expression and isolation of proteins

To express an enzyme of the present invention the above mentioned host cells transformed or transfected with a vector comprising a nucleic acid sequence encoding an enzyme of the present invention are typically cultured in a suitable nutrient medium under conditions permitting the production of the desired molecules, after which these are recovered from the cells, or the culture broth.

The medium used to culture the host cells may be any conventional medium suitable for growing the host cells, such as minimal or complex media containing appropriate supplements. Suitable media are available from commercial suppliers or may be prepared according to published recipes (e.g. in catalogues of the American Type Culture Collection). The media may be prepared using procedures known in the art (see, e.g., references for bacteria and yeast; Bennett, J.W. and LaSure, L., editors, More Gene Manipulations in Fungi, Academic Press, CA, 1991).

If the enzymes of the present invention are secreted into the nutrient medium, they may be recovered directly from the medium. If they are not secreted, they may be recovered from cell lysates. The enzymes of the present invention may be recovered from the culture medium by conventional procedures including separating the host cells from the medium by centrifugation or filtration, precipitating the proteinaceous components of the supernatant or filtrate by means of a salt, e.g. ammonium sulphate, purification by a variety of chromatographic procedures, e.g. ion exchange chromatography, gelfiltration chromatography, affinity chromatography, or the like, dependent on the enzyme in question.

The enzymes of the invention may be detected using methods known in the art that are specific for these proteins. These detection methods include use of specific antibodies, formation of a product, or disappearance of a substrate. For example, an enzyme assay may be used to determine the activity of the molecule. Procedures for determining various kinds of activity are known in the art.

The enzymes of the present invention may be purified by a variety of procedures known in the art including, but not limited to, chromatography (e.g., ion exchange, affinity, hydrophobic, chromatofocusing, and size exclusion), electrophoretic procedures (e.g., preparative isoelectric focusing (IEF), differential solubility (e.g., ammonium sulfate precipitation), or extraction (see, e.g., Protein Purification, J-C Janson and Lars Ryden, editors, VCH Publishers, New York, 1989).

When an expression vector comprising a DNA sequence encoding an enzyme of the present invention is transformed/transfected into a heterologous host cell it is possible to enable heterologous recombinant production of the enzyme. An advantage of using a heterologous host cell is that it is possible to make a highly purified enzyme composition, characterized in being free from homologous impurities, which are often present when a protein or peptide is expressed in a homologous host cell. In this context homologous impurities mean any impurity (e.g. other polypeptides than the enzyme of the invention) which originates from the homologous cell where the enzyme of the invention is originally obtained from.

DETERGENT APPLICATIONS

The enzyme of the invention may be added to and thus become a component of a detergent composition.

The detergent composition of the invention may for example be formulated as a hand or machine laundry detergent composition including a laundry additive composition suitable for pre-treatment of stained fabrics and a rinse added fabric softener composition, or be

formulated as a detergent composition for use in general household hard surface cleaning operations, or be formulated for hand or machine dishwashing operations.

In a specific aspect, the invention provides a detergent additive comprising the enzyme of the invention. The detergent additive as well as the detergent composition may comprise one or more other enzymes such as a protease, a lipase, a cutinase, an amylase, a carbohydrase, a cellulase, a pectinase, a mannanase, an arabinase, a galactanase, a xylanase, an oxidase, e.g., a laccase, and/or a peroxidase.

In general the properties of the chosen enzyme(s) should be compatible with the selected detergent, (i.e. pH-optimum, compatibility with other enzymatic and non-enzymatic ingredients, etc.), and the enzyme(s) should be present in effective amounts.

Proteases: Suitable proteases include those of animal, vegetable or microbial origin. Microbial origin is preferred. Chemically modified or protein engineered mutants are included. The protease may be a serine protease or a metallo protease, preferably an alkaline microbial protease or a trypsin-like protease. Examples of alkaline proteases are subtilisins, especially those derived from *Bacillus*, e.g., subtilisin Novo, subtilisin Carlsberg, subtilisin 309, subtilisin 147 and subtilisin 168 (described in WO 89/06279). Examples of trypsin-like proteases are trypsin (e.g. of porcine or bovine origin) and the *Fusarium* protease described in WO 89/06270 and WO 94/25583.

Examples of useful proteases are the variants described in WO 92/19729, WO 98/20115, WO 98/20116, and WO 98/34946, especially the variants with substitutions in one or more of the following positions: 27, 36, 57, 76, 87, 97, 101, 104, 120, 123, 167, 170, 194, 206, 218, 222, 224, 235 and 274.

Preferred commercially available protease enzymes include Alcalase™, Savinase™, Primase™, Duralase™, Esperase™, and Kannase™ (Novo Nordisk A/S), Maxatase™, Maxacal™, Maxapem™, Properase™, Purafect™, Purafect OxP™, FN2™, and FN3™ (Genencor International Inc.).

Lipases: Suitable lipases include those of bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Examples of useful lipases include lipases from *Humicola* (synonym *Thermomyces*), e.g. from *H. lanuginosa* (*T. lanuginosus*) as described in EP 258 068 and EP 305 216 or from *H. insolens* as described in WO 96/13580, a *Pseudomonas* lipase, e.g. from *P. alcaligenes* or *P. pseudoalcaligenes* (EP 218 272), *P. cepacia* (EP 331 376), *P. stutzeri* (GB 1,372,034), *P. fluorescens*, *Pseudomonas sp.* strain SD 705 (WO 95/06720 and WO 96/27002), *P. wisconsinensis* (WO 96/12012), a *Bacillus*

lipase, e.g. from *B. subtilis* (Dartois et al. (1993), Biochemica et Biophysica Acta, 1131, 253-360), *B. stearothermophilus* (JP 64/744992) or *B. pumilus* (WO 91/16422).

Other examples are lipase variants such as those described in WO 92/05249, WO 94/01541, EP 407 225, EP 260 105, WO 95/35381, WO 96/00292, WO 95/30744, WO 94/25578, WO 95/14783, WO 95/22615, WO 97/04079 and WO 97/07202.

Preferred commercially available lipase enzymes include Lipolase™ and Lipolase Ultra™ (Novo Nordisk A/S).

Amylases: Suitable amylases (α and/or β) include those of bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Amylases include, for example, α-amylases obtained from *Bacillus*, e.g. a special strain of *B. licheniformis*, described in more detail in GB 1,296,839.

Examples of useful amylases are the variants described in WO 94/02597, WO 94/18314, WO 96/23873, and WO 97/43424, especially the variants with substitutions in one or more of the following positions: 15, 23, 105, 106, 124, 128, 133, 154, 156, 181, 188, 190, 197, 202, 208, 209, 243, 264, 304, 305, 391, 408, and 444.

Commercially available amylases are Duramyl™, Termamyl™, Fungamyl™ and BAN™ (Novo Nordisk A/S), Rapidase™ and Purastar™ (from Genencor International Inc.).

Cellulases: Suitable cellulases include those of bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Suitable cellulases include cellulases from the genera *Bacillus, Pseudomonas, Humicola, Fusarium, Thielavia, Acremonium*, e.g. the fungal cellulases produced from *Humicola insolens, Myceliophthora thermophila* and *Fusarium oxysporum* disclosed in US 4,435,307, US 5,648,263, US 5,691,178, US 5,776,757 and WO 89/09259.

Especially suitable cellulases are the alkaline or neutral cellulases having colour care benefits. Examples of such cellulases are cellulases described in EP 0 495 257, EP 0 531 372, WO 96/11262, WO 96/29397, WO 98/08940. Other examples are cellulase variants such as those described in WO 94/07998, EP 0 531 315, US 5,457,046, US 5,686,593, US 5,763,254, WO 95/24471, WO 98/12307 and PCT/DK98/00299.

Commercially available cellulases include Celluzyme™, and Carezyme™ (Novo Nordisk A/S), Clazinase™, and Puradax HA™ (Genencor International Inc.), and KAC-500(B)™ (Kao Corporation).

Peroxidases/Oxidases: Suitable peroxidases/oxidases include those of plant, bacterial or fungal origin. Chemically modified or protein engineered mutants are included. Examples of useful peroxidases include peroxidases from *Coprinus*, e.g. from *C. cinereus*, and variants thereof as those described in WO 93/24618, WO 95/10602, and WO 98/15257.
Commercially available peroxidases include Guardzyme™ (Novo Nordisk A/S).

The detergent enzyme(s) may be included in a detergent composition by adding separate additives containing one or more enzymes, or by adding a combined additive comprising all of these enzymes. A detergent additive of the invention, i.e. a separate additive or a combined additive, can be formulated e.g. as a granulate, a liquid, a slurry, etc. Preferred detergent additive formulations are granulates, in particular non-dusting granulates, liquids, in particular stabilized liquids, or slurries.
Non-dusting granulates may be produced, e.g., as disclosed in US 4,106,991 and 4,661,452 and may optionally be coated by methods known in the art. Examples of waxy coating materials are poly(ethylene oxide) products (polyethyleneglycol, PEG) with mean molar weights of 1000 to 20000; ethoxylated nonylphenols having from 16 to 50 ethylene oxide units; ethoxylated fatty alcohols in which the alcohol contains from 12 to 20 carbon atoms and in which there are 15 to 80 ethylene oxide units; fatty alcohols; fatty acids; and mono- and di- and triglycerides of fatty acids. Examples of film-forming coating materials suitable for application by fluid bed techniques are given in GB 1483591. Liquid enzyme preparations may, for instance, be stabilized by adding a polyol such as propylene glycol, a sugar or sugar alcohol, lactic acid or boric acid according to established methods. Protected enzymes may be prepared according to the method disclosed in EP 238,216.

The detergent composition of the invention may be in any convenient form, e.g., a bar, a tablet, a powder, a granule, a paste or a liquid. A liquid detergent may be aqueous, typically containing up to 70 % water and 0-30 % organic solvent, or non-aqueous.

The detergent composition comprises one or more surfactants, which may be non-ionic including semi-polar and/or anionic and/or cationic and/or zwitterionic. The surfactants are typically present at a level of from 0.1% to 60% by weight.
When included therein the detergent will usually contain from about 1% to about 40% of an anionic surfactant such as linear alkylbenzenesulfonate, alpha-olefinsulfonate, alkyl sulfate (fatty alcohol sulfate), alcohol ethoxysulfate, secondary alkanesulfonate, alpha-sulfo fatty acid methyl ester, alkyl- or alkenylsuccinic acid or soap.

When included therein the detergent will usually contain from about 0.2% to about 40% of a non-ionic surfactant such as alcohol ethoxylate, nonylphenol ethoxylate, alkylpolyglycoside, alkyldimethylamineoxide, ethoxylated fatty acid monoethanolamide, fatty acid monoethanolamide, polyhydroxy alkyl fatty acid amide, or N-acyl N-alkyl derivatives of glucosamine ("glucamides").

The detergent may contain 0-65 % of a detergent builder or complexing agent such as zeolite, diphosphate, triphosphate, phosphonate, carbonate, citrate, nitrilotriacetic acid, ethylenediaminetetraacetic acid, diethylenetriaminepentaacetic acid, alkyl- or alkenylsuccinic acid, soluble silicates or layered silicates (e.g. SKS-6 from Hoechst).

The detergent may comprise one or more polymers. Examples are carboxymethylcellulose, poly(vinylpyrrolidone), poly (ethylene glycol), poly(vinyl alcohol), poly(vinylpyridine-N-oxide), poly(vinylimidazole), polycarboxylates such as polyacrylates, maleic/acrylic acid copolymers and lauryl methacrylate/acrylic acid copolymers.

The detergent may contain a bleaching system which may comprise a H_2O_2 source such as perborate or percarbonate which may be combined with a peracid-forming bleach activator such as tetraacetylethylenediamine or nonanoyloxybenzenesulfonate. Alternatively, the bleaching system may comprise peroxyacids of e.g. the amide, imide, or sulfone type.

The enzyme(s) of the detergent composition of the invention may be stabilized using conventional stabilizing agents, e.g., a polyol such as propylene glycol or glycerol, a sugar or sugar alcohol, lactic acid, boric acid, or a boric acid derivative, e.g., an aromatic borate ester, or a phenyl boronic acid derivative such as 4-formylphenyl boronic acid, and the composition may be formulated as described in e.g. WO 92/19709 and WO 92/19708.

The detergent may also contain other conventional detergent ingredients such as e.g. fabric conditioners including clays, foam boosters, suds suppressors, anti-corrosion agents, soil-suspending agents, anti-soil redeposition agents, dyes, bactericides, optical brighteners, hydrotropes, tarnish inhibitors, or perfumes.

In the detergent compositions any enzyme, in particular the enzyme of the invention, may be added in an amount corresponding to 0.01-100 mg of enzyme protein per litre of wash

liquor, preferably 0.05-5 mg of enzyme protein per litre of wash liquor, in particular 0.1-1 mg of enzyme protein per litre of wash liquor.

The enzyme of the invention may additionally be incorporated in the detergent formulations disclosed in WO 97/07202 which is hereby incorporated as reference.

MATERIALS AND METHODS

Textiles

Standard textile pieces are obtained from EMPA St. Gallen, Lerchfeldstrasse 5, CH-9014 St. Gallen, Switzerland. Especially type EMPA 116 (cotton textile stained with blood, milk and ink) and EMPA 117 (polyester/cotton textile stained with blood, milk and ink).

Method for producing a subtilase variant

The present invention provides a method of producing an isolated enzyme according to the invention, wherein a suitable host cell, which has been transformed with a DNA sequence encoding the enzyme, is cultured under conditions permitting the production of the enzyme, and the resulting enzyme is recovered from the culture.

When an expression vector comprising a DNA sequence encoding the enzyme is transformed into a heterologous host cell it is possible to enable heterologous recombinant production of the enzyme of the invention. Thereby it is possible to make a highly purified subtilase composition, characterized in being free from homologous impurities.

The medium used to culture the transformed host cells may be any conventional medium suitable for growing the host cells in question. The expressed subtilase may conveniently be secreted into the culture medium and may be recovered there-from by well-known procedures including separating the cells from the medium by centrifugation or filtration, precipitating proteinaceous components of the medium by means of a salt such as ammonium sulfate, followed by chromatographic procedures such as ion exchange chromatography, affinity chromatography, or the like.

EXAMPLE 1

Removal of ion-binding sites from BPN' like subtilases

The below mentioned regions in JP170 and TY145 have been selected for transfer from JP170 and TY145 to Savinase. By use of the molecular methods of preparing subtilase variants as described herein, the Savinase regions (BPN' numbering) are deleted and the

JP170 and TY145 regions are inserted instead. Since the Savinase regions are in contact with ion-binding sites, the purpose of the modifications is to remove the ion-binding site from Savinase.

Savinase	region A194-L196
JP170	region P209-P217 and
Savinase	region L75-L82
TY145	region H83-Y92,

alternatively the modification can be

Savinase	region A194-L196
JP170	region P209-P217 and
Savinase	region L75-L82
JP170	region N79-K83.

EXAMPLE 2

Purification and assessment of enzyme concentration

After fermentation, purification of subtilisin variants is accomplished using Hydrophobic Charge Induction Chromatography (HCIC) and subsequent vacuum filtration.

To capture the enzyme, the HCIC uses a cellulose matrix to which 4-Mercapto-Ethyl-Pyridine (4-MEP) is bound.

Beads of the cellulose matrix sized 80-100 µm are mixed with a media containing yeast and the transformed *B. subtilis* capable of secreting the subtilisin variants and incubated at pH 9.5 in Unifilter® microplates.

As 4-MEP is hydrophobic at pH > 7 and the subtilisin variants are hydrophobic at pH 9.5 a hydrophobic association is made between the secreted enzyme and the 4-MEP on the beads. After incubation the media and cell debris is removed by vacuum filtration while the beads and enzyme are kept on the filter.

To elute the enzyme from the beads the pH is now lowered by washing the filter with an elution buffer (pH 5). Hereby the enzymes part from the beads and can be retrieved from the buffer.

The concentration of the purified subtilisin enzyme variants is assessed by active site titration (AST).

The purified enzyme is incubated with the high affinity inhibitor CI-2A at different concentrations to inhibit a varying amount of the active sites. The protease and inhibitor binds to each other at a 1:1 ratio and accordingly the enzyme concentration can be directly related to the concentration of inhibitor, at which all protease is inactive. To measure the residual protease activity, a substrate (0.6 mM Suc-Ala-Ala-Pro-Phe-pNA in Tris/HCl buffer) is added after the incubation with inhibitor and during the following 4 minutes the development of the degradation product pNA (paranitrophenol) is measured periodically at 405 nm on an Elisa Reader.

EXAMPLE 3

Wash performance of detergent compositions comprising modified enzymes

Wash performance of detergent compositions comprising enzyme hybrids or enzyme variants of the present is tested at low washing temperature.

AMSA

The enzyme variants of the present application are tested using the Automatic Mechanical Stress Assay (AMSA). With the AMSA test the wash performance of a large quantity of small volume enzyme-detergent solutions can be examined. The AMSA plate has a number of slots for test solutions and a lid firmly squeezing the textile swatch to be washed against all the slot openings. During the washing time, the plate, test solutions, textile and lid are vigorously shaken to bring the test solution in contact with the textile and apply mechanical stress. For further description see WO 02/42740 especially the paragraph "Special method embodiments" at page 23-24.

The assay is conducted under the experimental conditions specified below:

Detergent base	Standard European detergent
Detergent dosage	1.5 g/l
Test solution volume	160 micro l
pH	10-10.5 adjusted with $NaHCO_3$
Wash time	12 minutes
Temperature	20°C

Water hardness	9°dH
Enzyme concentration in test solution	5 nM, 10 nM and 30 nM
Test material	EMPA 117

After washing the textile pieces are flushed in tap water and air-dried.

The performance of the enzyme variant is measured as the brightness of the colour of the textile samples washed with that specific enzyme variant. Brightness can also be expressed as the intensity of the light reflected from the textile sample when luminated with white light. When the textile is stained the intensity of the reflected light is lower, than that of a clean textile. Therefore the intensity of the reflected light can be used to measure wash performance of an enzyme variant.

Colour measurements are made with a professional flatbed scanner (*PFU DL2400pro*), which is used to capture an image of the washed textile samples. The scans are made with a resolution of 200 dpi and with an output colour dept of 24 bits. In order to get accurate results, the scanner is frequently calibrated with a *Kodak reflective IT8 target*.

To extract a value for the light intensity from the scanned images, a special designed software application is used (*Novozymes Color Vector Analyzer*). The program retrieves the 24 bit pixel values from the image and converts them into values for red, green and blue (RGB). The intensity value (Int) is calculated by adding the RGB values together as vectors and then taking the length of the resulting vector:

$$Int = \sqrt{r^2 + g^2 + b^2}$$

The wash performance (P) of the variants is calculated in accordance with the below formula:

$$P = Int(v) - Int(r)$$

where

Int(v) is the light intensity value of textile surface washed with enzyme variant and

Int(r) is the light intensity value of textile surface washed with the reference enzyme e.g. subtilisin 309 (BLSAVI).

Performance Scores (S) are summing up the performances (P) of the tested enzyme variants as:

S (2) which indicates that the variant performs better than the reference at all three

concentrations (5, 10 and 30 nM) and

S (1) which indicates that the variant performs better than the reference at one or two concentrations.

Mini wash assay

A millilitre scale wash performance assay is conducted under the following conditions:

Detergent base	Standard European detergent powder
Detergent dose	1.5 g/l
pH	"as is" in the current detergent solution and is not adjusted.
Wash time	14 min.
Temperature	20°C
Water hardness	9°dH, adjusted by adding $CaCl_2*2H_2O$; $MgCl_2*6H_2O$; $NaHCO_3$ (Ca^{2+}:Mg^{2+}:HCO^{3-} = 2:1:6) to milli-Q water.
Enzyme conc.	5 nM, 10 nM
Test system	125 ml glass beakers. Textile dipped in test solution. Continuously up and down, 50 times per minute
Textile/volume	1 textile piece (13 x 3 cm) in 50 ml test solution
Test material	EMPA 117 textile swatches

After wash the measurement of remission from the test material is done at 460 nm using a Zeiss MCS 521 VIS spectrophotometer. The measurements are done according to the manufacturer's protocol.

CLAIMS

1. A JP170 like subtilase which is at least 58% homologous to the sequence of SEQ ID NO:1, comprising the overall subtilisin fold and the following structural characteristics:

a) a twisted beta-sheet with 7 strands,

b) six alpha helices,

c) three ion-binding sites,

and not comprising the Strong and Weak ion-binding sites of the BPN' like subtilases, and with the exception of the subtilases JP170, KP1790, KP9860, KP43, Y, SD-521 and variants aam50090, aam50086, aam50085, aam50084, aam50083, aam50082, aam50081, aam50080 of EP 1209233.

2. The subtilase of claim 1, wherein the positions of said three ion-binding sites in the three-dimensional structure of the subtilase is defined by the distance to the c-alpha atoms of the three active site amino acid residues of the subtilases, that is Ser, His and Asp, and the c-alpha atom of the amino acid residue next to the active site Ser residue (next to Ser), wherein said distances between:

a) ion-binding site 1 and i) Asp c-alpha atom is 26.70-28.70Å, ii) His c-alpha atom is 22.10-24.10Å, iii) Ser c-alpha atom is 16.95-18.95Å, iv) next to Ser c-alpha atom is 15.30-17.30Å,

b) ion-binding site 2 and i) Asp c-alpha atom is 33.50-35.50Å, ii) His c-alpha atom is 37-39Å, iii) Ser c-alpha atom is 29.40-31.40Å, iv) next to Ser c-alpha atom is 30.70-32.70Å,

c) ion-binding site 3 and i) Asp c-alpha atom is 41.50-43.50Å, ii) His c-alpha atom is 42.90-44.90Å, iii) Ser c-alpha atom is 34.50-36.50Å, iv) next to Ser c-alpha atom is 35-37Å.

3. A subtilase according to claim 2 wherein the positions of the three ion-binding sites are defined by the distance to the c-alpha atoms of amino acid residues Asp30, His68, Ser254 and Met255 of SEQ ID NO:1 or by the distances to the c-alpha atoms of equivalent amino acid residues in another subtilase of the invention in accordance with claim 1, wherein the distance between

a) ion-binding site 1 and i) Asp c-alpha atom is 27.69Å, ii) His c-alpha atom is 23.12Å, iii) Ser c-alpha atom is 17.95Å, iv) next to Ser c-alpha atom is 16.34Å,

b) ion-binding site 2 and i) Asp c-alpha atom is 34.49Å, ii) His c-alpha atom is 38.03Å, iii)

Ser c-alpha atom is 30.41Å, iv) next to Ser c-alpha atom is 31.68Å,

c) ion-binding site 3 and i) Asp c-alpha atom is 42.48Å, ii) His c-alpha atom is 43.87Å, iii) Ser c-alpha atom is 35.51Å, iv) next to Ser c-alpha atom is 36.02Å,

and wherein the variation on the above mentioned distances are ±0.80Å, preferably ±0.70Å, more preferably ±0.60Å, more preferably ±0.50Å, more preferably ±0.40Å, or most preferably ±0.30Å.

4. A method of producing a variant of a parent JP170 like subtilase, the variant having at least one altered property as compared to the parent JP170 like subtilase, the method comprising:

a) modelling the parent JP170 like subtilase on the three-dimensional structure of a JP170 subtilase to produce a three-dimensional structure of the parent JP170 like subtilase;

b) identifying on the basis of the comparison in step a) at least one structural part of the parent JP170 subtilase, wherein an alteration in said structural part is predicted to result in an altered property;

c) modifying the nucleic acid sequence encoding the parent JP170 subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;

d) expressing the modified nucleic acid sequence in a host cell to produce the variant JP170 subtilase;

e) isolating the produced subtilase;

f) purifying the isolated subtilase and

g) recovering the purified subtilase.

5. A method according to claim 4, wherein the JP170 subtilase on which the parent JP170 subtilase is modelled in step a) is at least 58% homologous to SEQ ID NO:1, preferably at least 60% homologous, more preferably at least 65%, more preferably at least 70%, more preferably at least 75%, more preferably at least 80%, more preferably at least 85%, more preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more preferably at least 96%, more preferably at least 97%, more preferably at least 98% or even more preferably at least 99% homologous to the sequence of SEQ ID NO:1.

6. A method according to claim 4 or 5, wherein the JP170 subtilase on which the parent JP170 subtilase is modelled in step a) is defined in accordance with claim 3.

7. A method of producing a variant of a parent Subtilisin family subtilase, the variant having at least one altered property as compared to the parent Subtilisin family subtilase, the method comprising:

a) modelling the parent Subtilisin family subtilase on the three-dimensional structure of a Subtilisin family subtilase to produce a three-dimensional structure of the parent Subtilisin family subtilase;

b) comparing the three-dimensional structure obtained in step a) to the three-dimensional structure of a JP170 like subtilase;

c) identifying on the basis of the comparison in step b) at least one structural part of the parent Subtilisin family subtilase, wherein an alteration in said structural part is predicted to result in an altered property;

d) modifying the nucleic acid sequence encoding the parent Subtilisin family subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;

e) expressing the modified nucleic acid sequence in a host cell to produce the variant Subtilisin family subtilase,

f) isolating the produced subtilase,

g) purifying the isolated subtilase and

h) recovering the purified subtilase.

8. A method according to claim 7, wherein the Subtilisin family subtilase on which the parent Subtilisin family subtilase is modelled in step a) is at least 61% homologous to SEQ ID NO:4, preferably at least 63% homologous, preferably at least 65% homologous, more preferably at least 70%, more preferably at least 74%, more preferably at least 80%, more preferably at least 83%, more preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more preferably at least 96%, more preferably at least 97%, more preferably at least 98% or even more preferably at least 99% homologous to the sequence of SEQ ID NO:4.

9. A method according to any of claim 7 and 8, wherein the JP170 subtilase of step b) is defined in accordance with claim 3.

10. A method according to any of claims 7-9, wherein the JP170 subtilase in step b) is at least 58% homologous with the sequence of SEQ ID NO:1, preferably at least 60% homologous, more preferably at least 65%, more preferably at least 70%, more preferably at least 75%, more preferably at least 80%, more preferably at least 85%, more preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more preferably at least 96%, more preferably at least 97%, more preferably at least 98% or even more preferably at least 99% homologous to the sequence of SEQ ID NO:1.

11. A method of producing a variant of a parent JP170 like subtilase, the variant having at least one altered property as compared to the parent JP170 like subtilase, the method comprising:

a) modelling the parent JP170 like subtilase on the three-dimensional structure of a JP170 like subtilase to produce a three-dimensional structure of the parent JP170 like subtilase;
b) comparing the three-dimensional structure obtained in step a) to the three-dimensional structure of a Subtilisin family subtilase;
c) identifying on the basis of the comparison in step b) at least one structural part of the parent JP170 like subtilase, wherein an alteration in said structural part is predicted to result in an altered property;
d) modifying the nucleic acid sequence encoding the parent JP170 like subtilase to produce a nucleic acid sequence encoding deletion or substitution of one or more amino acids at a position corresponding to said structural part, or an insertion of one or more amino acid residues in positions corresponding to said structural part;
e) expressing the modified nucleic acid sequence in a host cell to produce the variant JP170 like subtilase;
f) isolating the produced subtilase;
g) purifying the isolated subtilase and
h) recovering the purified subtilase.

12. A method according to claim 11, wherein the Subtilisin family subtilase of step b) is at least 61% homologous to SEQ ID NO:4, preferably at least 63% homologous, preferably at

least 65% homologous, more preferably at least 70%, more preferably at least 74%, more preferably at least 80%, more preferably at least 83%, more preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more preferably at least 96%, more preferably at least 97%, more preferably at least 98% or even more preferably at least 99% homologous to the sequence of SEQ ID NO:4.

13. A method according to any of claim 11 and 12, wherein the parent JP170 like subtilase is defined in accordance with claim 3.

14. A method according to any of claims 11-13, wherein the parent JP170 like subtilase is at least 58% homologous with the sequence of SEQ ID NO:1, preferably at least 60% homologous, more preferably at least 65%, more preferably at least 70%, more preferably at least 75%, more preferably at least 80%, more preferably at least 85%, more preferably at least 90%, more preferably at least 91%, more preferably at least 92%, more preferably at least 93%, more preferably at least 94%, more preferably at least 95%, more preferably at least 96%, more preferably at least 97%, more preferably at least 98% or even more preferably at least 99% homologous to the sequence of SEQ ID NO:1.

15. A variant subtilase comprising an alteration in one or more positions located at a distance of not more than 10Å to one of the ion-binding sites of JP170, wherein the positions, as specified in SEQ ID NO:1, located at a distance of not more than 10Å to:

a) ion-binding site 1 are: 183, 184, 185, 186, 187, 188, 189, 191, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 224 and 225,
b) ion-binding site 2 are: 378, 379, 380, 381, 382, 383, 384, 385, 386, 387, 388, 389, 390, 391, 392 and 393,
c) ion-binding site 3 are: 348, 350, 352, 363, 364, 365, 366, 367, 368, 369, 370, 380, 381, 382, 383, 391, 392, 393, 394, 395, 396, 397, 398, 399, 400, 414, 415, 416, 417, 418, 419, 420.

16. A subtilase variant according to claim 15 comprising one or more of the substitutions: S193Q,Y; H200D,N; H200D,N+D196N; N390D; N391D; G394N,Q,F,Y,S and W392S,N,Q.

17. A JP170 like subtilase variant comprising the introduction of a ion-binding site corresponding to the Strong ion-binding site of the BPN' like family subtilases, wherein said vari-

ant has a deletion of or in the region N79-N82 of SEQ ID NO:1 and subsequent insertion of one or more amino acid residues, preferably insertion of the sequence LNNSIQV followed by the substitution A45D,N and optionally the substitutions E44P,T and/or R47Q.

18. A JP170 like subtilase variant in which one or more ion-binding sites have been removed, wherein said variant comprises deletion of or in the region N186-N199 of SEQ ID NO:1 and subsequent insertion of one or more amino acid residues, preferably insertion of the sequence SSN, and preferably further comprising one or both of the substitutions I7Q and V3Y.

19. A BPN' like subtilase variant in which the ion-binding sites has been removed, wherein said variant comprises:

a) deletion of or in the region A194-L196 (Savinase in BPN' numbering) or a corresponding region in another BPN' like subtilase and insertion of three or more amino acid residues, preferably insertion of P209-P217 from JP170 or a corresponding region in another JP170 like subtilase and
deletion of or in the region L75-L82 (Savinase in BPN' numbering) or a corresponding region in said other BPN' like subtilase and insertion of one or more amino acid residues, preferably insertion of H83-Y92 from TY145 or a corresponding region in another TY145 like subtilase or

b) deletion of or in the region A194-L196 (Savinase in BPN' numbering) or a corresponding region in another BPN' like subtilase and insertion of three or more amino acid residues, preferably insertion of P209-P217 from JP170 or a corresponding region in another JP170 like subtilase and
deletion of or in the L75-L82 (Savinase in BPN' numbering) or a corresponding region in said other BPN' like subtilase and insertion of one or more amino acid residues, preferably insertion of N79-K83 from JP170 or a corresponding region in another JP170 like subtilase.

20. A JP170 like subtilase variant comprising an alteration in one or more of the following positions:
13, 14, 15, 16, 17, 18,
37, 38, 39, 40, 41, 42, 43,
47, 48, 49, 50,
57, 58, 59,

96, 97, 98, 99, 100, 101, 102, 103,
131, 132, 133, 134,
152, 153
162, 163, 164, 165, 166,
188, 189, 190, 191, 192, 193, 194, 195,
210
234, 235, 236, 237, 238, 239, 240, 241, 242, 243, 244, 245, 246,
372, 373, 374, 375, 376, 377, 378,
387, 388, 389, 390, 391, 392,
406, 407 and
419.

21. A JP170 like subtilase variant comprising an alteration in one or more of the following positions:
37, 38, 39, 40, 41, 42,
57, 58, 59, 60,
66, 67,
98, 99, 100, 101, 102, 103,
107, 108, 109, 110, 111,
188, 189, 190, 191, 192, 193,
236, 237, 238, 239, 240,
326, 327, 328, 329, 330, 331, 332,
337, 338, 339, 340, 341, 342,
355, 356, 357, 358, 359, 360,
372, 373, 374, 375, 376, 377,
384, 385, 386, 387, 388,
404, 405, 406, 407, 408, 409, 410, 411.

22. A subtilase variant according to claim 21 comprising one or more of the modifications:
W240H,Y; G355A,S; S356T,N; T357N,Q,D,E,P; T358S; A359S,T,N,Q and S360T,N.

23. A variant subtilase comprising an alteration in one or more positions which are within a distance of 10Å from a CI2 inhibitor which is bound to the active site of JP170, wherein the positions, as specified in SEQ ID NO:1 are:

29, 30, 31, 32, 64, 65, 66, 67, 68, 69, 70, 71, 72, 93, 96, 97, 98, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 113, 114, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 138, 139, 140, 141, 144, 157, 174, 180, 181, 182, 183, 191, 193, 194, 202, 203, 204, 205, 206, 207, 211, 223, 224, 225, 226, 234, 235, 236, 237, 238, 239, 240, 241, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258,
preferably comprising the substitution W129L.

24. A JP170 like subtilase variant comprising one or more disulfide bridges introduced by one or more of the following modifications: G21C/A86C, V26C/A265C, G57C/G105C, G74C/A229C, Q111C/Y143C, G160C/S170C, A286C/V349C, A27C/A122C, A45C/G78C, V72C/P258C, G78C/A229C, D98C/G104C, Q111C/Y147C, G135C/G167C, R142C/P354C, V144C/A178C, G182C/P217C, A183C/G223C, A195C/Y225C, F271C/P279C, A287C/A430C, A293C/S310C, E322C/S428C, S324C/A332C, S327C/P424C, D352C/N397C, G255C/T362C, G291C/S314C, A4C/P222C and A27C/V117C, wherein the positions correspond to the positions in SEQ ID NO:1

25. A JP170 like subtilase variant comprising an alteration in one or more of the positions N76, N316, L381, K246, K9, K313 and K83, preferably comprising one or more of the substitutions N79D, N316D, L381D, K246R, K9R, K313R and K83R of SEQ ID NO:1.

26. A JP170 like subtilase variant comprising an alteration in one or more of the positions 22, 44, 110, 139, 140, 166, 198, 201, 203, 231, 282, 356, 357 and 378, preferably comprising one or more of the substitutions: Q22P, E44P, L110P, T139P, D140P, S166P I198P, V201P, Q203P, S231P, S282P, S356P, T357P and K378P.

27. A JP170 like subtilase variant comprising a deletion of the region 311-433, preferably deletion of positions 317-433 or 315-433, further comprising one or more of the substitutions L283N,Q; A290S,N and W306H,Y,K.

28. A subtilase variant according to claim 27, comprising

a) deletion of positions 317-433 and the substitutions L283N, A290S and W306H, or

b) deletion of region 315-433 and the substitutions L283N, A290S and W306H.

29. An isolated nucleic acid sequence comprising a nucleic acid sequence, which encodes for the subtilase variant defined or produced in any of the preceding claims.

30. An isolated nucleic acid sequence according to claim 29, wherein the nucleic acid sequence is selected form the group consisting of:

a) a nucleic acid sequence encoding an enzyme having at least 58% homology with the amino acid sequence shown in SEQ ID NO:1, and

b) a nucleic acid sequence which hybridizes under low stringency conditions, preferably under medium stringency conditions, in particular under high stringency conditions, with a complementary strand of the nucleic acid sequence encoding an enzyme having at least 58% homology with the amino acid sequence shown in SEQ ID NO:1, or

c) a subsequence of any of a) or b) of at least 100 nucleotides.

31. An isolated nucleic acid construct comprising a nucleic acid sequence as defined in any of claims 29-30, operably linked to one or more control sequences capable of directing the expression of the polypeptide in a suitable expression host.

32. A recombinant host cell comprising the nucleic acid construct of claim 31.

33. A method for producing the variant defined in any of the preceding claims, the method comprising:

a) cultivating the recombinant host cell of claim 32 under conditions conducive to the production of the subtilase variant; and

b) recovering the variant.

34. A detergent composition comprising a JP170 like subtilase variant or a BPN' like subtilase variant.

35. Use of a JP170 like subtilase variant or a BPN' like subtilase variant in cleaning or washing applications.

ABSTRACT

The present invention relates to methods for producing variants of a parent JP170 subtilase and of a parent BPN' subtilase and to JP170 and BPN' variants having altered properties as compared to the parent JP170/BPN' subtilase.

Figure 1. Alignment of 3D sequences of protease JP170 (mature sequence from App. 1), SD-521 (aam50084 from EP 1209233) and protease Y (aay44619 from WO99/67370).

```
                1                                                   50
aam50084    NDVARGIVKA DVAQNNYGLY GQGQVVAVAD TGLDTGRNDS SMHEAFRGKI
aay44619    NDVARGIVKA DVAQNNYGLY GQGQLVAVAD TGLDTGRNDS SMHEAFRGKI
JP170       NDVARGIVKA DVAQNNFGLY GQGQIVAVAD TGLDTGRNDS SMHEAFRGKI

               51                                                  100
aam50084    TALYALGRTN NANDPNGHGT HVAGSVLGNA LNKGMAPQAN LVFQSIMDSS
aay44619    TALYALGRTN NASDPNGHGT HVAGSVLGNA LNKGMAPQAN LVFQSIMDSS
JP170       TALYALGRTN NANDPNGHGT HVAGSVLGNA TNKGMAPQAN LVFQSIMDSG

              101                                                  150
aam50084    GGLGGLPSNL NTLFSQAWNA GARIHTNSWG APVNGAYTAN SRQVDEYVRN
aay44619    GGLGGLPSNL NTLFSQAWNA GARIHTNSWG APVNGAYTAN SRQVDEYVRN
JP170       GGLGGLPANL QTLFSQAYSA GARIHTNSWG APVNGAYTTD SRNVDDYVRK

              151                                                  200
aam50084    NDMTVLFAAG NEGPNSGTIS APGTAKNAIT VGATENYRPS FGSLADNPNH
aay44619    NDMTVLFAAG NEGPNSGTIS APGTAKNAIT VGATENYRPS FGSIADNPNH
JP170       NDMTILFAAG NEGPGSGTIS APGTAKNAIT VGATENLRPS FGSYADNINH

              201                                                  250
aam50084    IAQFSSRGAT RDGRIKPDVT APGTFILSAR SSLAPDSSFW ANYNSKYAYM
aay44619    IAQFSSRGAT RDGRIKPDVT APGTFILSAR SSLAPDSSFW ANYNSKYAYM
JP170       VAQFSSRGPT RDGRIKPDVM APGTYILSAR SSLAPDSSFW ANHDSKYAYM

              251                                                  300
aam50084    GGTSMATPIV AGNVAQLREH FIKNRGITPK PSLIKAALIA GATDVGLGYP
aay44619    GGTSMATPIV AGNVAQLREH FIKNRGITPK PSLIKAALIA GATDVGLGYP
JP170       GGTSMATPIV AGNVAQLREH FVKNRGVTPK PSLLKAALIA GAADVGLGFP

              301                                                  350
aam50084    SGDQGWGRVT LDKSLNVAYV NEATALATGQ KATYSFQAQA GKPLKISLVW
aay44619    SGDQGWGRVT LDKSLNVAYV NEATALATGQ KATYSFQAQA GKPLKISLVW
JP170       NGNQGWGRVT LDKSLNVAFV NETSPLSTSQ KATYSFTAQA GKPLKISLVW

              351                                                  400
aam50084    TDAPGSTTAS YTLVNDLDLV ITAPNGQKYV GNDFSYPYDN NWDGRNNVEN
aay44619    TDAPGSTTAS YTLVNDLDLV ITAPNGQKYV GNDFSYPYDN NWDGRNNVEN
JP170       SDAPGSTTAS LTLVNDLDLV ITAPNGTKYV GNDFTAPYDN NWDGRNNVEN

              401                                 433
aam50084    VFINAPQSGT YTIEVQAYNV PSGPQRFSLA IVH
aay44619    VFINAPQSGT YIIEVQAYNV PSGPQRFSLA IVH
JP170       VFINAPQSGT YTVEVQAYNV PVSPQTFSLA IVH
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Figure 2, Superposition of JP170 and Savinase 3D structures, with indication of calcium binding sites. JP170: light structure and three ion-binding sites. Savinase: dark structure and two ion-binding sites.

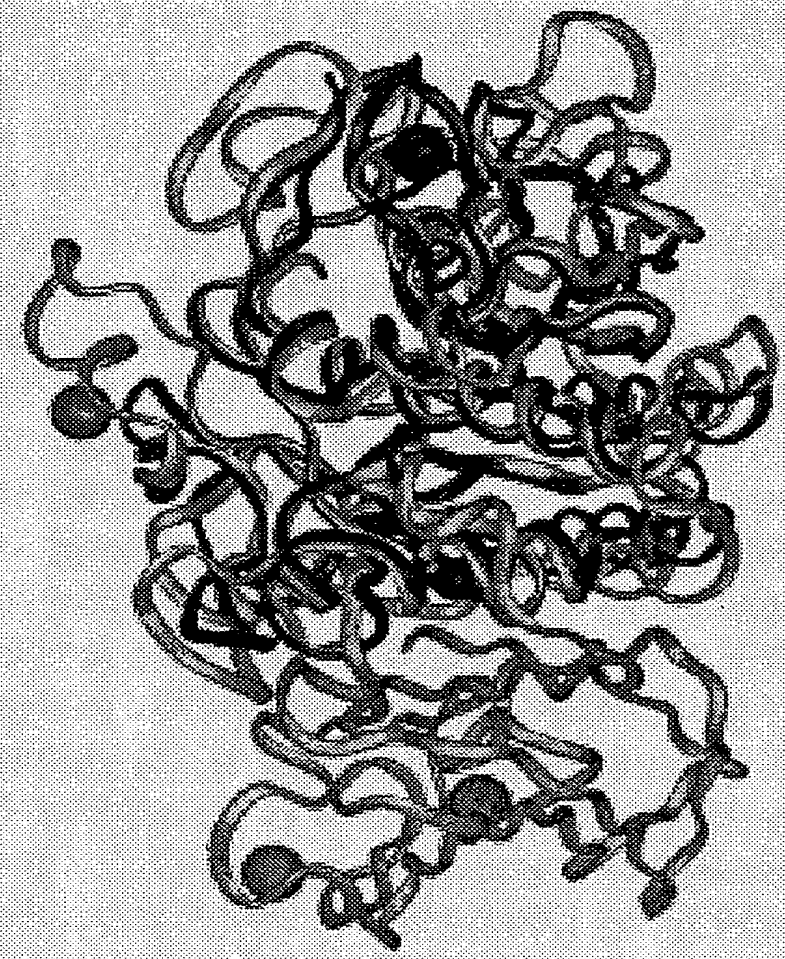

Figure 3, Matrix of homology between subtilases pertaining to the JP170, TY145 and BPN' subgroups. The sequences are identified by sequence database accession numbers:

00: aam50084; Subtilase derived from *Bacillus sp.* strain SD-521

0: aaw89547; Subtilase derived from *Bacillus sp.* JP170

1: q45681; Subtilase derived from *B. subtilis* (BSTA41)

2: p28842; Psychrophilic subtilisin derived from Antarctic *Bacillus* strain (BSTA39)

3: abb77095; Subtilase derived from *Bacillus sp.* (TY145)

4: p00783; Subtilase derived from *Bacillus subtilis var. amylosacchariticus* (BSAMY)

5: p29142; Subtilase derived from *Bacillus stearothermophilus* (BSSJ)

6: p35835; Subtilase derived from *Bacillus subtilis var. natto.* (BSNAT)

7: p07518; Subtilase derived from *Bacillus pumilus (B. mesentericus)* (BPMES)

8: p00782; Subtilase derived from *Bacillus amyloliquefaciens* (BPN')

9: p00780; Subtilase derived from *Bacillus licheniformis* (BLSCAR)

10: p41363; Subtilase derived from *Bacillus halodurans* (BHSAH)

11: aaw62222; Subtilase derived from *Bacillus lentus* (BLS147)

12: p29600; Subtilase derived from *Bacillus lentus* (BLSAVI, BLS309)

13: p27693; Subtilase derived from *Bacillus alcalophilus* (BAALKP)

14: q99405; Subtilase derived from *Bacillus sp.* strain KSM-K16 (BSKSMK)

15: p29599; Subtilase derived from *Bacillus lentus* (BLSUBL).

	00	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
00 aam50084	100	94	53	53	51	53	53	52	52	53	55	52	52	51	51	51	50
0 aaw89547		100	52	53	53	51	51	49	50	51	51	50	54	54	53	54	54
1 q45681			100	93	76	51	50	51	55	52	54	58	58	59	57	60	60
2 p28842				100	75	52	52	52	56	53	55	58	58	61	58	62	61
3 abb77095					100	60	60	60	58	60	62	58	57	59	59	62	59
4 p00783						100	99	99	97	91	76	63	69	74	66	74	74
5 p29142							100	99	97	90	76	69	74	66	74	74	56
6 p35835								100	98	91	77	63	69	74	66	74	74
7 p07518									100	88	79	69	67	74	74	74	74
8 p00782										100	77	66	71	74	67	74	74
9 p00780											100	64	69	74	67	73	73
10 p41363												100	99	76	72	76	76
11 aaw62222													100	76	76	76	76
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13 p27693															100	99	99
14 q99405																100	98
15 p29599																	100

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Leu Asp Thr Gly Arg Asn Asp Ser Ser Met His Glu Ala Phe Arg Gly
        35                  40                  45

Lys Ile Thr Ala Leu Tyr Ala Leu Gly Arg Thr Asn Asn Ala Asn Asp
    50                  55                  60

Pro Asn Gly His Gly Thr His Val Ala Gly Ser Val Leu Gly Asn Ala
65                  70                  75                  80

Thr Asn Lys Gly Met Ala Pro Gln Ala Asn Leu Val Phe Gln Ser Ile
                85                  90                  95

Met Asp Ser Gly Gly Gly Leu Gly Gly Leu Pro Ala Asn Leu Gln Thr
            100                 105                 110

Leu Phe Ser Gln Ala Tyr Ser Ala Gly Ala Arg Ile His Thr Asn Ser
        115                 120                 125

Trp Gly Ala Pro Val Asn Gly Ala Tyr Thr Thr Asp Ser Arg Asn Val
    130                 135                 140

Asp Asp Tyr Val Arg Lys Asn Asp Met Thr Ile Leu Phe Ala Ala Gly
145                 150                 155                 160

Asn Glu Gly Pro Gly Ser Gly Thr Ile Ser Ala Pro Gly Thr Ala Lys
                165                 170                 175
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180 185 190

Ser Tyr Ala Asp Asn Ile Asn His Val Ala Gln Phe Ser Ser Arg Gly
195 200 205

Pro Thr Arg Asp Gly Arg Ile Lys Pro Asp Val Met Ala Pro Gly Thr
210 215 220

Tyr Ile Leu Ser Ala Arg Ser Ser Leu Ala Pro Asp Ser Ser Phe Trp
225 230 235 240

Ala Asn His Asp Ser Lys Tyr Ala Tyr Met Gly Gly Thr Ser Met Ala
245 250 255

Thr Pro Ile Val Ala Gly Asn Val Ala Gln Leu Arg Glu His Phe Val
260 265 270

Lys Asn Arg Gly Val Thr Pro Lys Pro Ser Leu Leu Lys Ala Ala Leu
275 280 285

Ile Ala Gly Ala Ala Asp Val Gly Leu Gly Phe Pro Asn Gly Asn Gln
290 295 300

Gly Trp Gly Arg Val Thr Leu Asp Lys Ser Leu Asn Val Ala Phe Val
305 310 315 320

Asn Glu Thr Ser Pro Leu Ser Thr Ser Gln Lys Ala Thr Tyr Ser Phe
325 330 335

Thr Ala Gln Ala Gly Lys Pro Leu Lys Ile Ser Leu Val Trp Ser Asp
340 345 350

Ala Pro Gly Ser Thr Thr Ala Ser Leu Thr Leu Val Asn Asp Leu Asp
355 360 365

Leu Val Ile Thr Ala Pro Asn Gly Thr Lys Tyr Val Gly Asn Asp Phe
370 375 380

Thr Ala Pro Tyr Asp Asn Asn Trp Asp Gly Arg Asn Asn Val Glu Asn
385 390 395 400

Val Phe Ile Asn Ala Pro Gln Ser Gly Thr Tyr Thr Val Glu Val Gln
405 410 415

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            20                  25                  30

Leu Asp Thr Gly Arg Asn Asp Ser Ser Met His Glu Ala Phe Arg Gly
        35                  40                  45

Lys Ile Thr Ala Leu Tyr Ala Leu Gly Arg Thr Asn Asn Ala Ser Asp
    50                  55                  60

Pro Asn Gly His Gly Thr His Val Ala Gly Ser Val Leu Gly Asn Ala
65                  70                  75                  80

Leu Asn Lys Gly Met Ala Pro Gln Ala Asn Leu Val Phe Gln Ser Ile
                85                  90                  95

Met Asp Ser Ser Gly Gly Leu Gly Gly Leu Pro Ser Asn Leu Asn Thr
            100                 105                 110

Leu Phe Ser Gln Ala Trp Asn Ala Gly Ala Arg Ile His Thr Asn Ser
        115                 120                 125

Trp Gly Ala Pro Val Asn Gly Ala Tyr Thr Ala Asn Ser Arg Gln Val
    130                 135                 140

Asp Glu Tyr Val Arg Asn Asn Asp Met Thr Val Leu Phe Ala Ala Gly
145                 150                 155                 160

Asn Glu Gly Pro Asn Ser Gly Thr Ile Ser Ala Pro Gly Thr Ala Lys
                165                 170                 175

Asn Ala Ile Thr Val Gly Ala Thr Glu Asn Tyr Arg Pro Ser Phe Gly
            180                 185                 190

Ser Ile Ala Asp Asn Pro Asn His Ile Ala Gln Phe Ser Ser Arg Gly
        195                 200                 205

Ala Thr Arg Asp Gly Arg Ile Lys Pro Asp Val Thr Ala Pro Gly Thr
    210                 215                 220
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Phe Ile Leu Ser Ala Arg Ser Ser Leu Ala Pro Asp Ser Ser Phe Trp
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Thr Pro Ile Val Ala Gly Asn Val Ala Gln Leu Arg Glu His Phe Ile
260 265 270

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275 280 285

Ile Ala Gly Ala Thr Asp Val Gly Leu Gly Tyr Pro Ser Gly Asp Gln
290 295 300

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305 310 315 320

Asn Glu Ala Thr Ala Leu Ala Thr Gly Gln Lys Ala Thr Tyr Ser Phe
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340 345 350

Ala Pro Gly Ser Thr Thr Ala Ser Tyr Thr Leu Val Asn Asp Leu Asp
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370 375 380

Ser Tyr Pro Tyr Asp Asn Asn Trp Asp Gly Arg Asn Asn Val Glu Asn
385 390 395 400

Val Phe Ile Asn Ala Pro Gln Ser Gly Thr Tyr Ile Ile Glu Val Gln
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            20                  25                  30

Leu Asp Thr Gly Arg Asn Asp Ser Ser Met His Glu Ala Phe Arg Gly
        35                  40                  45

Lys Ile Thr Ala Leu Tyr Ala Leu Gly Arg Thr Asn Asn Ala Asn Asp
    50                  55                  60

Pro Asn Gly His Gly Thr His Val Ala Gly Ser Val Leu Gly Asn Ala
65                  70                  75                  80

Leu Asn Lys Gly Met Ala Pro Gln Ala Asn Leu Val Phe Gln Ser Ile
                85                  90                  95

Met Asp Ser Ser Gly Gly Leu Gly Gly Leu Pro Ser Asn Leu Asn Thr
            100                 105                 110

Leu Phe Ser Gln Ala Trp Asn Ala Gly Ala Arg Ile His Thr Asn Ser
        115                 120                 125

Trp Gly Ala Pro Val Asn Gly Ala Tyr Thr Ala Asn Ser Arg Gln Val
    130                 135                 140

Asp Glu Tyr Val Arg Asn Asn Asp Met Thr Val Leu Phe Ala Ala Gly
145                 150                 155                 160

Asn Glu Gly Pro Asn Ser Gly Thr Ile Ser Ala Pro Gly Thr Ala Lys
                165                 170                 175

Asn Ala Ile Thr Val Gly Ala Thr Glu Asn Tyr Arg Pro Ser Phe Gly
            180                 185                 190

Ser Leu Ala Asp Asn Pro Asn His Ile Ala Gln Phe Ser Ser Arg Gly
        195                 200                 205

Ala Thr Arg Asp Gly Arg Ile Lys Pro Asp Val Thr Ala Pro Gly Thr
    210                 215                 220

Phe Ile Leu Ser Ala Arg Ser Ser Leu Ala Pro Asp Ser Ser Phe Trp
225                 230                 235                 240

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Asn Glu Ala Thr Ala Leu Ala Thr Gly Gln Lys Ala Thr Tyr Ser Phe
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Gln Ala Gln Ala Gly Lys Pro Leu Lys Ile Ser Leu Val Trp Thr Asp
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Gly Thr His Val Ala Gly Thr Val Ala Ala Leu Asn Asn Ser Ile Gly
65                  70                  75                  80

Val Leu Gly Val Ala Pro Ser Ala Ser Leu Tyr Ala Val Lys Val Leu
                85                  90                  95

Gly Ala Asp Gly Ser Gly Gln Tyr Ser Trp Ile Ile Asn Gly Ile Glu
            100                 105                 110

Trp Ala Ile Ala Asn Asn Met Asp Val Ile Asn Met Ser Leu Gly Gly
        115                 120                 125

Pro Ser Gly Ser Ala Ala Leu Lys Ala Ala Val Asp Lys Ala Val Ala
    130                 135                 140

Ser Gly Val Val Val Val Ala Ala Ala Gly Asn Glu Gly Thr Ser Gly
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Ser Ser Ser Thr Val Gly Tyr Pro Gly Lys Tyr Pro Ser Val Ile Ala
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Val Gly Ala Val Asp Ser Ser Asn Gln Arg Ala Ser Phe Ser Ser Val
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Gly Pro Glu Leu Asp Val Met Ala Pro Gly Val Ser Ile Gln Ser Thr
        195                 200                 205

Leu Pro Gly Asn Lys Tyr Gly Ala Tyr Asn Gly Thr Ser Met Ala Ser
    210                 215                 220

Pro His Val Ala Gly Ala Ala Ala Leu Ile Leu Ser Lys His Pro Asn
225                 230                 235                 240

Trp Thr Asn Thr Gln Val Arg Ser Ser Leu Glu Asn Thr Thr Thr Lys
                245                 250                 255

Leu Gly Asp Ser Phe Tyr Tyr Gly Lys Gly Leu Ile Asn Val Gln Ala
            260                 265                 270

Ala Ala Gln
        275
```

APPENDIX 1

```
REMARK Complex of JP170 and CI2A inhibitor
REMARK Contents of asymmetric unit subtilisin 2x (433 a.a. x 2)
REMARK CI2A inhibitor 2x (a.a. 16 - 83 and 21 - 83)
REMARK small peptide (autodigestion product, a.a. KPSLL, 280 - 284)
REMARK Ca ions 6x, H2O 1115 x
REMARK
REMARK Crystallization conditions: (AMB) Hanging drop vapour diffusion
REMARK method where the drop consists of 2 µl of 15 - 20 mg.ml-1
REMARK protein concentration, 10 mM Na cacodylate - HCl buffer, pH 6.5
REMARK and 1 µl of the well solution, 20% w/v PEG 4000, 0.1 M Hepes
REMARK buffer, pH 7.5, 10% v/v isopropanol.
HEADER    ----                                        XX-XXX-XX   xxxx
COMPND    ---
REMARK   3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : REFMAC 5.1.24
REMARK   3   AUTHORS     : MURSHUDOV,VAGIN,DODSON
REMARK   3
REMARK   3    REFINEMENT TARGET : MAXIMUM LIKELIHOOD
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) :   1.90
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) :  19.96
REMARK   3   DATA CUTOFF            (SIGMA(F)) : NONE
REMARK   3   COMPLETENESS FOR RANGE        (%) :  76.65
REMARK   3   NUMBER OF REFLECTIONS             :   59444
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD           : NULL
REMARK   3   FREE R VALUE TEST SET SELECTION   : NULL
REMARK   3   R VALUE      (WORKING + TEST SET) : 0.12256
REMARK   3   R VALUE            (WORKING SET) :  0.12256
REMARK   3   FREE R VALUE                      : NULL
REMARK   3   FREE R VALUE TEST SET SIZE   (%)  : NULL
REMARK   3   FREE R VALUE TEST SET COUNT       : NULL
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           :      20
REMARK   3   BIN RESOLUTION RANGE HIGH           :   1.901
REMARK   3   BIN RESOLUTION RANGE LOW            :   1.950
REMARK   3   REFLECTION IN BIN     (WORKING SET) :     940
REMARK   3   BIN R VALUE           (WORKING SET) :   0.149
REMARK   3   BIN FREE R VALUE SET COUNT          :       0
REMARK   3   BIN FREE R VALUE                    : -999.000
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   ALL ATOMS                 :    8694
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) :  16.479
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) :    0.05
REMARK   3    B22 (A**2) :    0.06
REMARK   3    B33 (A**2) :   -0.11
REMARK   3    B12 (A**2) :    0.00
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REMARK   3    B13 (A**2) :      0.00
REMARK   3    B23 (A**2) :      0.00
REMARK   3
REMARK   3  ESTIMATED OVERALL COORDINATE ERROR.
REMARK   3   ESU BASED ON R VALUE                                (A):    0.151
REMARK   3   ESU BASED ON FREE R VALUE                           (A): NULL
REMARK   3   ESU BASED ON MAXIMUM LIKELIHOOD                     (A):    0.052
REMARK   3   ESU FOR B VALUES BASED ON MAXIMUM LIKELIHOOD (A**2):    1.828
REMARK   3
REMARK   3 CORRELATION COEFFICIENTS.
REMARK   3   CORRELATION COEFFICIENT FO-FC      :   0.969
REMARK   3   CORRELATION COEFFICIENT FO-FC FREE : NULL
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES         COUNT    RMS     WEIGHT
REMARK   3   BOND LENGTHS REFINED ATOMS        (A):  7733 ; 0.014 ; 0.021
REMARK   3   BOND LENGTHS OTHERS               (A):  6857 ; 0.001 ; 0.020
REMARK   3   BOND ANGLES REFINED ATOMS   (DEGREES): 10540 ; 1.478 ; 1.936
REMARK   3   BOND ANGLES OTHERS          (DEGREES): 15972 ; 0.815 ; 3.000
REMARK   3   TORSION ANGLES, PERIOD 1    (DEGREES):   997 ;15.784 ; 5.000
REMARK   3   CHIRAL-CENTER RESTRAINTS       (A**3):  1197 ; 0.106 ; 0.200
REMARK   3   GENERAL PLANES REFINED ATOMS      (A):  8819 ; 0.007 ; 0.020
REMARK   3   GENERAL PLANES OTHERS             (A):  1500 ; 0.008 ; 0.020
REMARK   3   NON-BONDED CONTACTS REFINED ATOMS (A):  1552 ; 0.221 ; 0.300
REMARK   3   NON-BONDED CONTACTS OTHERS        (A):  8282 ; 0.265 ; 0.300
REMARK   3   NON-BONDED TORSION OTHERS         (A):  4417 ; 0.089 ; 0.500
REMARK   3   H-BOND (X...Y) REFINED ATOMS      (A):  1391 ; 0.198 ; 0.500
REMARK   3   POTENTIAL METAL-ION REFINED ATOMS (A):    25 ; 0.145 ; 0.500
REMARK   3   SYMMETRY VDW REFINED ATOMS        (A):    10 ; 0.129 ; 0.300
REMARK   3   SYMMETRY VDW OTHERS               (A):    57 ; 0.268 ; 0.300
REMARK   3   SYMMETRY H-BOND REFINED ATOMS     (A):    87 ; 0.272 ; 0.500
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     COUNT    RMS     WEIGHT
REMARK   3   MAIN-CHAIN BOND REFINED ATOMS (A**2):  4985 ; 0.697 ; 1.500
REMARK   3   MAIN-CHAIN ANGLE REFINED ATOMS (A**2):  8031 ; 1.205 ; 2.000
REMARK   3   SIDE-CHAIN BOND REFINED ATOMS  (A**2):  2746 ; 1.963 ; 3.000
REMARK   3   SIDE-CHAIN ANGLE REFINED ATOMS (A**2):  2509 ; 3.180 ; 4.500
REMARK   3
REMARK   3  NCS RESTRAINTS STATISTICS
REMARK   3   NUMBER OF NCS GROUPS : NULL
REMARK   3
REMARK   3
REMARK   3  TLS DETAILS
REMARK   3   NUMBER OF TLS GROUPS  : NULL
REMARK   3
REMARK   3
REMARK   3  BULK SOLVENT MODELLING.
REMARK   3   METHOD USED : BABINET MODEL WITH MASK
REMARK   3   PARAMETERS FOR MASK CALCULATION
REMARK   3   VDW PROBE RADIUS   :   1.40
REMARK   3   ION PROBE RADIUS   :   0.80
REMARK   3   SHRINKAGE RADIUS   :   0.80
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS:
REMARK   3  HYDROGENS HAVE BEEN ADDED IN THE RIDING POSITIONS
REMARK   3
CISPEP   1 GLY A  163     PRO A  164                      0.00
CISPEP   2 ALA A  171     PRO A  172                      0.00
CISPEP   3 PHE A  191     GLY A  192                      0.00
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CISPEP    4 ASN A  199     HIS A  200                    0.00
CISPEP    5 GLY A  208     PRO A  209                    0.00
CISPEP    6 LYS A  216     PRO A  217                    0.00
CISPEP    7 ASP A  236     SER A  237                    0.00
CISPEP    8 ASP A  244     SER A  245                    0.00
CISPEP    9 PHE A  299     PRO A  300                    0.00
CISPEP   10 SER A  327     THR A  328                    0.00
CISPEP   11 ALA A  386     PRO A  387                    0.00
CISPEP   12 GLU A  414     VAL A  415                    0.00
CISPEP   13 GLY A  423     PRO A  424                    0.00
LINK              ASN B 316                   LYS B 318                 gap
LINK              GLU B 330                   ALA B 332                 gap
LINK              LEU B 337                   LYS B 340                 gap
LINK              GLU D 330                   ALA D 332                 gap
LINK              LEU D 337                   LYS D 340                 gap
CISPEP   14 GLY C  163     PRO C  164                    0.00
CISPEP   15 ALA C  171     PRO C  172                    0.00
CISPEP   16 PHE C  191     GLY C  192                    0.00
CISPEP   17 ASN C  199     HIS C  200                    0.00
CISPEP   18 GLY C  208     PRO C  209                    0.00
CISPEP   19 LYS C  216     PRO C  217                    0.00
CISPEP   20 ASP C  236     SER C  237                    0.00
CISPEP   21 ASP C  244     SER C  245                    0.00
CISPEP   22 PHE C  299     PRO C  300                    0.00
CISPEP   23 SER C  327     THR C  328                    0.00
CISPEP   24 ALA C  386     PRO C  387                    0.00
CISPEP   25 GLU C  414     VAL C  415                    0.00
CISPEP   26 GLY C  423     PRO C  424                    0.00
CRYST1   58.387  151.411   64.054  90.00 117.11  90.00 P 1 21 1
SCALE1      0.017127  0.000000  0.008768        0.00000
SCALE2      0.000000  0.006605  0.000000        0.00000
SCALE3      0.000000  0.000000  0.017539        0.00000
HETATM    1  N   ASN A   1      18.066  20.808  -3.996  1.00 14.87      A    N
HETATM    2  C9  ASN A   1      18.461  22.053  -3.689  1.00 14.47      A    C
HETATM    3  O10 ASN A   1      19.168  22.251  -2.661  1.00 13.33      A    O
HETATM    4  O11 ASN A   1      18.108  23.029  -4.423  1.00 14.69      A    O
HETATM    5  CA  ASN A   1      18.499  19.635  -3.189  1.00 14.35      A    C
HETATM    6  CB  ASN A   1      18.164  18.329  -3.883  1.00 14.69      A    C
HETATM    7  CG  ASN A   1      16.670  18.063  -4.031  1.00 14.08      A    C
HETATM    8  ND2 ASN A   1      16.271  17.100  -5.019  1.00 12.20      A    N
HETATM    9  OD1 ASN A   1      15.768  18.701  -3.206  1.00 14.76      A    O
HETATM   10  C   ASN A   1      19.990  19.659  -2.890  1.00 14.84      A    C
HETATM   11  O   ASN A   1      20.353  19.313  -1.601  1.00 14.20      A    O
ATOM     12  N   ASP A   2      20.881  19.935  -3.834  1.00 15.84      A    N
ATOM     13  CA  ASP A   2      22.306  19.835  -3.520  1.00 16.82      A    C
ATOM     14  CB  ASP A   2      23.178  20.088  -4.763  1.00 17.53      A    C
ATOM     15  CG  ASP A   2      23.121  18.947  -5.783  1.00 18.18      A    C
ATOM     16  OD1 ASP A   2      22.652  17.811  -5.493  1.00 20.58      A    O
ATOM     17  OD2 ASP A   2      23.544  19.106  -6.931  1.00 22.02      A    O
ATOM     18  C   ASP A   2      22.712  20.816  -2.413  1.00 17.23      A    C
ATOM     19  O   ASP A   2      23.671  20.562  -1.703  1.00 18.17      A    O
ATOM     20  N   VAL A   3      22.018  21.952  -2.304  1.00 17.05      A    N
ATOM     21  CA  VAL A   3      22.374  22.945  -1.311  1.00 16.07      A    C
ATOM     22  CB  VAL A   3      21.974  24.356  -1.701  1.00 16.60      A    C
ATOM     23  CG1 VAL A   3      22.327  25.323  -0.560  1.00 16.25      A    C
ATOM     24  CG2 VAL A   3      22.676  24.770  -3.003  1.00 18.81      A    C
ATOM     25  C   VAL A   3      21.749  22.565   0.033  1.00 15.65      A    C
ATOM     26  O   VAL A   3      22.431  22.603   1.090  1.00 14.41      A    O
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ATOM	27	N	ALA	A	4	20.497	22.119	-0.012	1.00	13.75	A	N
ATOM	28	CA	ALA	A	4	19.824	21.664	1.196	1.00	14.03	A	C
ATOM	29	CB	ALA	A	4	18.388	21.260	0.881	1.00	13.78	A	C
ATOM	30	C	ALA	A	4	20.544	20.512	1.876	1.00	14.28	A	C
ATOM	31	O	ALA	A	4	20.548	20.406	3.110	1.00	14.07	A	O
ATOM	32	N	ARG	A	5	21.093	19.617	1.064	1.00	13.74	A	N
ATOM	33	CA	ARG	A	5	21.807	18.445	1.553	1.00	14.95	A	C
ATOM	34	CB	ARG	A	5	22.395	17.709	0.349	1.00	15.61	A	C
ATOM	35	CG	ARG	A	5	23.452	16.639	0.631	1.00	17.28	A	C
ATOM	36	CD	ARG	A	5	23.873	15.945	-0.672	1.00	20.73	A	C
ATOM	37	NE	ARG	A	5	24.802	14.852	-0.459	1.00	21.95	A	N
ATOM	38	CZ	ARG	A	5	26.128	14.986	-0.513	1.00	24.69	A	C
ATOM	39	NH1	ARG	A	5	26.687	16.173	-0.793	1.00	25.62	A	N
ATOM	40	NH2	ARG	A	5	26.898	13.933	-0.290	1.00	22.96	A	N
ATOM	41	C	ARG	A	5	22.918	18.840	2.515	1.00	14.83	A	C
ATOM	42	O	ARG	A	5	23.135	18.195	3.546	1.00	14.86	A	O
ATOM	43	N	GLY	A	6	23.641	19.897	2.166	1.00	15.33	A	N
ATOM	44	CA	GLY	A	6	24.677	20.416	3.044	1.00	15.34	A	C
ATOM	45	C	GLY	A	6	24.094	21.124	4.257	1.00	15.01	A	C
ATOM	46	O	GLY	A	6	24.609	20.980	5.362	1.00	14.62	A	O
ATOM	47	N	ILE	A	7	23.018	21.879	4.062	1.00	14.44	A	N
ATOM	48	CA	ILE	A	7	22.411	22.613	5.168	1.00	13.98	A	C
ATOM	49	CB	ILE	A	7	21.266	23.505	4.698	1.00	13.68	A	C
ATOM	50	CG1	ILE	A	7	21.813	24.676	3.864	1.00	13.35	A	C
ATOM	51	CD1	ILE	A	7	20.794	25.294	2.972	1.00	14.08	A	C
ATOM	52	CG2	ILE	A	7	20.511	24.072	5.873	1.00	12.51	A	C
ATOM	53	C	ILE	A	7	21.970	21.664	6.305	1.00	15.04	A	C
ATOM	54	O	ILE	A	7	22.273	21.906	7.469	1.00	13.35	A	O
ATOM	55	N	VAL	A	8	21.320	20.558	5.952	1.00	15.03	A	N
ATOM	56	CA	VAL	A	8	20.795	19.628	6.969	1.00	14.89	A	C
ATOM	57	CB	VAL	A	8	19.419	19.047	6.545	1.00	14.63	A	C
ATOM	58	CG1	VAL	A	8	18.472	20.135	6.246	1.00	14.63	A	C
ATOM	59	CG2	VAL	A	8	19.526	18.151	5.333	1.00	15.54	A	C
ATOM	60	C	VAL	A	8	21.770	18.511	7.356	1.00	14.75	A	C
ATOM	61	O	VAL	A	8	21.438	17.645	8.168	1.00	15.23	A	O
ATOM	62	N	LYS	A	9	22.983	18.568	6.804	1.00	14.02	A	N
ATOM	63	CA	LYS	A	9	24.061	17.627	7.118	1.00	14.55	A	C
ATOM	64	CB	LYS	A	9	24.374	17.560	8.621	1.00	15.28	A	C
ATOM	65	CG	LYS	A	9	24.553	18.888	9.299	1.00	18.34	A	C
ATOM	66	CD	LYS	A	9	25.757	19.608	8.810	1.00	23.66	A	C
ATOM	67	CE	LYS	A	9	26.025	20.904	9.618	1.00	28.33	A	C
ATOM	68	NZ	LYS	A	9	27.283	21.559	9.079	1.00	31.91	A	N
ATOM	69	C	LYS	A	9	23.798	16.226	6.616	1.00	13.77	A	C
ATOM	70	O	LYS	A	9	24.391	15.256	7.132	1.00	13.96	A	O
ATOM	71	N	ALA	A	10	22.979	16.109	5.569	1.00	13.98	A	N
ATOM	72	CA	ALA	A	10	22.816	14.830	4.886	1.00	14.34	A	C
ATOM	73	CB	ALA	A	10	21.649	14.866	3.848	1.00	14.47	A	C
ATOM	74	C	ALA	A	10	24.141	14.437	4.205	1.00	14.55	A	C
ATOM	75	O	ALA	A	10	24.409	13.264	4.015	1.00	13.73	A	O
ATOM	76	N	ASP	A	11	24.967	15.423	3.860	1.00	16.04	A	N
ATOM	77	CA	ASP	A	11	26.278	15.153	3.265	1.00	17.11	A	C
ATOM	78	CB	ASP	A	11	26.899	16.419	2.667	1.00	17.53	A	C
ATOM	79	CG	ASP	A	11	27.059	17.547	3.680	1.00	19.89	A	C
ATOM	80	OD1	ASP	A	11	27.845	18.461	3.375	1.00	23.81	A	O
ATOM	81	OD2	ASP	A	11	26.434	17.635	4.773	1.00	20.19	A	O
ATOM	82	C	ASP	A	11	27.219	14.489	4.285	1.00	17.57	A	C
ATOM	83	O	ASP	A	11	27.941	13.540	3.947	1.00	17.08	A	O
ATOM	84	N	VAL	A	12	27.153	14.945	5.528	1.00	17.31	A	N

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ATOM     85  CA  VAL A  12      27.926  14.338   6.607  1.00 17.86      A    C
ATOM     86  CB  VAL A  12      27.850  15.193   7.893  1.00 18.12      A    C
ATOM     87  CG1 VAL A  12      28.577  14.533   9.081  1.00 18.00      A    C
ATOM     88  CG2 VAL A  12      28.385  16.633   7.631  1.00 19.36      A    C
ATOM     89  C   VAL A  12      27.428  12.898   6.835  1.00 18.14      A    C
ATOM     90  O   VAL A  12      28.233  11.956   6.925  1.00 18.38      A    O
ATOM     91  N   ALA A  13      26.117  12.696   6.870  1.00 17.13      A    N
ATOM     92  CA  ALA A  13      25.572  11.353   7.076  1.00 17.08      A    C
ATOM     93  CB  ALA A  13      24.070  11.400   7.101  1.00 17.00      A    C
ATOM     94  C   ALA A  13      26.044  10.394   5.981  1.00 17.57      A    C
ATOM     95  O   ALA A  13      26.472   9.237   6.254  1.00 16.79      A    O
ATOM     96  N   GLN A  14      25.934  10.862   4.740  1.00 17.24      A    N
ATOM     97  CA  GLN A  14      26.420  10.107   3.582  1.00 17.55      A    C
ATOM     98  CB  GLN A  14      25.972  10.825   2.309  1.00 17.74      A    C
ATOM     99  CG  GLN A  14      24.485  10.673   2.031  1.00 17.61      A    C
ATOM    100  CD  GLN A  14      23.995  11.535   0.887  1.00 20.02      A    C
ATOM    101  OE1 GLN A  14      24.788  11.949   0.028  1.00 19.60      A    O
ATOM    102  NE2 GLN A  14      22.679  11.789   0.850  1.00 19.07      A    N
ATOM    103  C   GLN A  14      27.949   9.876   3.576  1.00 18.95      A    C
ATOM    104  O   GLN A  14      28.413   8.729   3.489  1.00 18.61      A    O
ATOM    105  N   ASN A  15      28.730  10.950   3.658  1.00 19.73      A    N
ATOM    106  CA  ASN A  15      30.185  10.847   3.469  1.00 20.71      A    C
ATOM    107  CB  ASN A  15      30.828  12.222   3.244  1.00 20.45      A    C
ATOM    108  CG  ASN A  15      30.404  12.869   1.959  1.00 22.21      A    C
ATOM    109  OD1 ASN A  15      30.098  12.201   0.976  1.00 25.39      A    O
ATOM    110  ND2 ASN A  15      30.390  14.182   1.953  1.00 23.97      A    N
ATOM    111  C   ASN A  15      30.865  10.185   4.653  1.00 20.49      A    C
ATOM    112  O   ASN A  15      31.705   9.362   4.469  1.00 21.06      A    O
ATOM    113  N   ASN A  16      30.495  10.559   5.869  1.00 21.00      A    N
ATOM    114  CA  ASN A  16      31.148  10.056   7.073  1.00 21.90      A    C
ATOM    115  CB  ASN A  16      31.205  11.146   8.136  1.00 22.29      A    C
ATOM    116  CG  ASN A  16      32.100  12.313   7.751  1.00 26.21      A    C
ATOM    117  OD1 ASN A  16      32.261  13.260   8.533  1.00 32.71      A    O
ATOM    118  ND2 ASN A  16      32.672  12.268   6.567  1.00 28.57      A    N
ATOM    119  C   ASN A  16      30.491   8.811   7.692  1.00 21.95      A    C
ATOM    120  O   ASN A  16      31.152   8.065   8.404  1.00 22.21      A    O
ATOM    121  N   PHE A  17      29.203   8.578   7.438  1.00 20.66      A    N
ATOM    122  CA  PHE A  17      28.550   7.392   8.003  1.00 20.24      A    C
ATOM    123  CB  PHE A  17      27.415   7.815   8.938  1.00 21.09      A    C
ATOM    124  CG  PHE A  17      27.890   8.591  10.134  1.00 19.81      A    C
ATOM    125  CD1 PHE A  17      28.110   7.953  11.348  1.00 24.93      A    C
ATOM    126  CE1 PHE A  17      28.556   8.679  12.459  1.00 25.33      A    C
ATOM    127  CZ  PHE A  17      28.779  10.016  12.344  1.00 23.90      A    C
ATOM    128  CE2 PHE A  17      28.564  10.651  11.155  1.00 22.65      A    C
ATOM    129  CD2 PHE A  17      28.111   9.936  10.052  1.00 20.02      A    C
ATOM    130  C   PHE A  17      28.061   6.385   6.977  1.00 19.13      A    C
ATOM    131  O   PHE A  17      27.607   5.336   7.337  1.00 20.18      A    O
ATOM    132  N   GLY A  18      28.205   6.685   5.692  1.00 17.84      A    N
ATOM    133  CA  GLY A  18      27.740   5.790   4.640  1.00 17.25      A    C
ATOM    134  C   GLY A  18      26.220   5.654   4.496  1.00 16.27      A    C
ATOM    135  O   GLY A  18      25.755   4.667   3.948  1.00 14.47      A    O
ATOM    136  N   LEU A  19      25.453   6.651   4.955  1.00 15.24      A    N
ATOM    137  CA  LEU A  19      23.980   6.550   5.007  1.00 14.35      A    C
ATOM    138  CB  LEU A  19      23.456   7.222   6.270  1.00 14.71      A    C
ATOM    139  CG  LEU A  19      24.013   6.680   7.569  1.00 15.58      A    C
ATOM    140  CD1 LEU A  19      23.691   7.633   8.721  1.00 16.09      A    C
ATOM    141  CD2 LEU A  19      23.417   5.294   7.793  1.00 15.86      A    C
ATOM    142  C   LEU A  19      23.305   7.203   3.820  1.00 13.82      A    C
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ATOM    143  O   LEU A  19      23.183   8.427   3.775  1.00 13.96      A    O
ATOM    144  N   TYR A  20      22.874   6.400   2.854  1.00 13.81      A    N
ATOM    145  CA  TYR A  20      22.156   6.917   1.714  1.00 14.22      A    C
ATOM    146  CB  TYR A  20      22.841   6.499   0.386  1.00 14.36      A    C
ATOM    147  CG  TYR A  20      24.254   7.034   0.241  1.00 14.09      A    C
ATOM    148  CD1 TYR A  20      25.351   6.353   0.792  1.00 16.48      A    C
ATOM    149  CE1 TYR A  20      26.661   6.858   0.663  1.00 16.91      A    C
ATOM    150  CZ  TYR A  20      26.859   8.041  -0.034  1.00 18.57      A    C
ATOM    151  OH  TYR A  20      28.126   8.567  -0.171  1.00 21.21      A    O
ATOM    152  CE2 TYR A  20      25.788   8.735  -0.575  1.00 17.45      A    C
ATOM    153  CD2 TYR A  20      24.495   8.217  -0.461  1.00 16.03      A    C
ATOM    154  C   TYR A  20      20.715   6.433   1.702  1.00 14.55      A    C
ATOM    155  O   TYR A  20      19.994   6.688   0.723  1.00 14.48      A    O
ATOM    156  N   GLY A  21      20.297   5.710   2.746  1.00 14.18      A    N
ATOM    157  CA  GLY A  21      18.947   5.172   2.802  1.00 14.23      A    C
ATOM    158  C   GLY A  21      18.749   3.775   2.207  1.00 14.56      A    C
ATOM    159  O   GLY A  21      17.611   3.315   2.054  1.00 13.53      A    O
ATOM    160  N   GLN A  22      19.838   3.084   1.883  1.00 14.57      A    N
ATOM    161  CA  GLN A  22      19.722   1.726   1.334  1.00 14.82      A    C
ATOM    162  CB  GLN A  22      21.095   1.130   0.978  1.00 15.45      A    C
ATOM    163  CG  GLN A  22      21.054  -0.151   0.150  1.00 17.91      A    C
ATOM    164  CD  GLN A  22      20.669  -1.376   0.976  1.00 21.79      A    C
ATOM    165  OE1 GLN A  22      20.892  -1.414   2.185  1.00 22.42      A    O
ATOM    166  NE2 GLN A  22      20.091  -2.379   0.317  1.00 23.11      A    N
ATOM    167  C   GLN A  22      19.011   0.831   2.331  1.00 14.04      A    C
ATOM    168  O   GLN A  22      19.341   0.824   3.516  1.00 14.39      A    O
ATOM    169  N   GLY A  23      18.019   0.110   1.836  1.00 14.26      A    N
ATOM    170  CA  GLY A  23      17.236  -0.859   2.628  1.00 14.81      A    C
ATOM    171  C   GLY A  23      15.957  -0.245   3.176  1.00 14.12      A    C
ATOM    172  O   GLY A  23      15.086  -0.948   3.718  1.00 14.17      A    O
ATOM    173  N   GLN A  24      15.836   1.077   3.057  1.00 13.54      A    N
ATOM    174  CA  GLN A  24      14.620   1.773   3.500  1.00 13.27      A    C
ATOM    175  CB  GLN A  24      14.963   3.090   4.182  1.00 12.64      A    C
ATOM    176  CG  GLN A  24      15.806   2.945   5.450  1.00 13.46      A    C
ATOM    177  CD  GLN A  24      15.150   2.100   6.505  1.00 15.72      A    C
ATOM    178  OE1 GLN A  24      14.015   2.387   6.921  1.00 14.73      A    O
ATOM    179  NE2 GLN A  24      15.839   1.026   6.927  1.00 13.89      A    N
ATOM    180  C   GLN A  24      13.619   2.022   2.352  1.00 13.19      A    C
ATOM    181  O   GLN A  24      14.005   2.126   1.184  1.00 13.48      A    O
ATOM    182  N   ILE A  25      12.324   2.066   2.692  1.00 13.28      A    N
ATOM    183  CA  ILE A  25      11.280   2.319   1.720  1.00 13.25      A    C
ATOM    184  CB  ILE A  25      10.404   1.077   1.507  1.00 13.64      A    C
ATOM    185  CG1 ILE A  25      11.267  -0.108   1.030  1.00 15.44      A    C
ATOM    186  CD1 ILE A  25      10.508  -1.518   0.962  1.00 14.73      A    C
ATOM    187  CG2 ILE A  25       9.303   1.387   0.503  1.00 13.37      A    C
ATOM    188  C   ILE A  25      10.447   3.491   2.209  1.00 13.24      A    C
ATOM    189  O   ILE A  25       9.884   3.430   3.285  1.00 12.93      A    O
ATOM    190  N   VAL A  26      10.438   4.573   1.432  1.00 12.43      A    N
ATOM    191  CA  VAL A  26       9.656   5.754   1.737  1.00 12.49      A    C
ATOM    192  CB  VAL A  26      10.480   7.034   1.585  1.00 12.90      A    C
ATOM    193  CG1 VAL A  26       9.671   8.231   2.059  1.00 11.57      A    C
ATOM    194  CG2 VAL A  26      11.796   6.928   2.395  1.00 15.53      A    C
ATOM    195  C   VAL A  26       8.465   5.823   0.804  1.00 12.34      A    C
ATOM    196  O   VAL A  26       8.601   5.646  -0.418  1.00 11.99      A    O
ATOM    197  N   ALA A  27       7.297   6.044   1.387  1.00 12.40      A    N
ATOM    198  CA  ALA A  27       6.080   6.289   0.624  1.00 12.49      A    C
ATOM    199  CB  ALA A  27       4.846   5.650   1.284  1.00 11.39      A    C
ATOM    200  C   ALA A  27       5.892   7.790   0.546  1.00 12.17      A    C
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ATOM    201  O   ALA A  27       6.077   8.501   1.526  1.00 11.39      A    O
ATOM    202  N   VAL A  28       5.540   8.243  -0.643  1.00 11.79      A    N
ATOM    203  CA  VAL A  28       5.168   9.612  -0.910  1.00 11.63      A    C
ATOM    204  CB  VAL A  28       6.054  10.176  -2.003  1.00 11.56      A    C
ATOM    205  CG1 VAL A  28       5.629  11.625  -2.440  1.00 12.77      A    C
ATOM    206  CG2 VAL A  28       7.514  10.079  -1.594  1.00 11.95      A    C
ATOM    207  C   VAL A  28       3.729   9.580  -1.458  1.00 11.23      A    C
ATOM    208  O   VAL A  28       3.470   8.936  -2.459  1.00 10.72      A    O
ATOM    209  N   ALA A  29       2.817  10.294  -0.831  1.00 10.64      A    N
ATOM    210  CA  ALA A  29       1.468  10.435  -1.365  1.00 11.32      A    C
ATOM    211  CB  ALA A  29       0.441  10.151  -0.298  1.00 11.33      A    C
ATOM    212  C   ALA A  29       1.326  11.842  -1.909  1.00 11.35      A    C
ATOM    213  O   ALA A  29       1.404  12.826  -1.161  1.00 11.19      A    O
ATOM    214  N   ASP A  30       1.186  11.937  -3.229  1.00 11.71      A    N
ATOM    215  CA  ASP A  30       1.266  13.221  -3.917  1.00 11.52      A    C
ATOM    216  CB  ASP A  30       2.718  13.715  -3.958  1.00 11.37      A    C
ATOM    217  CG  ASP A  30       2.802  15.221  -3.852  1.00 12.40      A    C
ATOM    218  OD1 ASP A  30       3.385  15.726  -2.871  1.00 12.15      A    O
ATOM    219  OD2 ASP A  30       2.226  15.973  -4.682  1.00 14.39      A    O
ATOM    220  C   ASP A  30       0.665  13.113  -5.327  1.00 12.41      A    C
ATOM    221  O   ASP A  30       0.068  12.086  -5.671  1.00 12.89      A    O
ATOM    222  N   THR A  31       0.811  14.162  -6.151  1.00 12.52      A    N
ATOM    223  CA  THR A  31      -0.004  14.263  -7.353  1.00 11.62      A    C
ATOM    224  CB  THR A  31       0.302  15.554  -8.182  1.00 11.72      A    C
ATOM    225  OG1 THR A  31       1.709  15.702  -8.423  1.00 11.44      A    O
ATOM    226  CG2 THR A  31      -0.099  16.789  -7.424  1.00 11.85      A    C
ATOM    227  C   THR A  31       0.126  13.041  -8.225  1.00 12.59      A    C
ATOM    228  O   THR A  31      -0.868  12.341  -8.494  1.00 12.63      A    O
ATOM    229  N   GLY A  32       1.360  12.810  -8.665  1.00 12.03      A    N
ATOM    230  CA  GLY A  32       1.694  11.788  -9.617  1.00 12.81      A    C
ATOM    231  C   GLY A  32       3.202  11.763  -9.729  1.00 13.22      A    C
ATOM    232  O   GLY A  32       3.885  12.607  -9.135  1.00 12.83      A    O
ATOM    233  N   LEU A  33       3.711  10.813 -10.501  1.00 13.41      A    N
ATOM    234  CA  LEU A  33       5.139  10.622 -10.678  1.00 13.86      A    C
ATOM    235  CB  LEU A  33       5.625   9.397  -9.899  1.00 13.74      A    C
ATOM    236  CG  LEU A  33       7.148   9.234  -9.900  1.00 14.12      A    C
ATOM    237  CD1 LEU A  33       7.768  10.273  -8.964  1.00 13.99      A    C
ATOM    238  CD2 LEU A  33       7.497   7.818  -9.437  1.00 15.42      A    C
ATOM    239  C   LEU A  33       5.517  10.505 -12.151  1.00 13.89      A    C
ATOM    240  O   LEU A  33       5.374   9.444 -12.765  1.00 14.14      A    O
ATOM    241  N   ASP A  34       6.009  11.612 -12.696  1.00 14.55      A    N
ATOM    242  CA  ASP A  34       6.455  11.701 -14.087  1.00 14.62      A    C
ATOM    243  CB  ASP A  34       7.899  11.201 -14.224  1.00 14.72      A    C
ATOM    244  CG  ASP A  34       8.516  11.532 -15.598  1.00 15.30      A    C
ATOM    245  OD1 ASP A  34       9.260  10.694 -16.148  1.00 14.31      A    O
ATOM    246  OD2 ASP A  34       8.268  12.602 -16.207  1.00 17.33      A    O
ATOM    247  C   ASP A  34       5.470  11.016 -15.060  1.00 14.94      A    C
ATOM    248  O   ASP A  34       4.297  11.415 -15.124  1.00 15.39      A    O
ATOM    249  N   THR A  35       5.927  10.013 -15.816  1.00 16.25      A    N
ATOM    250  CA  THR A  35       5.083   9.340 -16.813  1.00 16.50      A    C
ATOM    251  CB  THR A  35       5.912   8.471 -17.786  1.00 17.03      A    C
ATOM    252  OG1 THR A  35       6.700   7.514 -17.051  1.00 17.34      A    O
ATOM    253  CG2 THR A  35       6.922   9.300 -18.593  1.00 17.53      A    C
ATOM    254  C   THR A  35       4.005   8.437 -16.229  1.00 17.26      A    C
ATOM    255  O   THR A  35       3.111   7.992 -16.946  1.00 15.49      A    O
ATOM    256  N   GLY A  36       4.104   8.104 -14.948  1.00 16.59      A    N
ATOM    257  CA  GLY A  36       3.094   7.259 -14.360  1.00 16.76      A    C
ATOM    258  C   GLY A  36       3.308   5.802 -14.660  1.00 17.58      A    C
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ATOM    259  O   GLY A  36       2.432   4.984 -14.383  1.00 17.55      A    O
ATOM    260  N   ARG A  37       4.473   5.465 -15.200  1.00 18.31      A    N
ATOM    261  CA  ARG A  37       4.748   4.091 -15.575  1.00 19.42      A    C
ATOM    262  CB  ARG A  37       4.763   3.940 -17.088  1.00 20.37      A    C
ATOM    263  CG  ARG A  37       3.436   4.298 -17.742  1.00 23.71      A    C
ATOM    264  CD  ARG A  37       3.283   3.740 -19.140  1.00 31.29      A    C
ATOM    265  NE  ARG A  37       4.324   4.233 -20.024  1.00 34.29      A    N
ATOM    266  CZ  ARG A  37       4.322   5.434 -20.575  1.00 38.63      A    C
ATOM    267  NH1 ARG A  37       5.331   5.792 -21.361  1.00 39.90      A    N
ATOM    268  NH2 ARG A  37       3.305   6.273 -20.362  1.00 40.23      A    N
ATOM    269  C   ARG A  37       6.072   3.661 -14.998  1.00 19.41      A    C
ATOM    270  O   ARG A  37       7.065   4.354 -15.150  1.00 18.12      A    O
ATOM    271  N   ASN A  38       6.067   2.506 -14.334  1.00 19.47      A    N
ATOM    272  CA  ASN A  38       7.254   1.998 -13.703  1.00 20.37      A    C
ATOM    273  CB  ASN A  38       6.917   1.215 -12.431  1.00 20.71      A    C
ATOM    274  CG  ASN A  38       8.161   0.841 -11.658  1.00 21.12      A    C
ATOM    275  OD1 ASN A  38       9.248   1.337 -11.968  1.00 18.41      A    O
ATOM    276  ND2 ASN A  38       8.023  -0.072 -10.684  1.00 20.60      A    N
ATOM    277  C   ASN A  38       7.984   1.134 -14.700  1.00 21.21      A    C
ATOM    278  O   ASN A  38       7.918  -0.099 -14.638  1.00 21.03      A    O
ATOM    279  N   ASP A  39       8.659   1.806 -15.625  1.00 21.69      A    N
ATOM    280  CA  ASP A  39       9.363   1.158 -16.718  1.00 23.22      A    C
ATOM    281  CB  ASP A  39       8.405   0.839 -17.882  1.00 23.19      A    C
ATOM    282  CG  ASP A  39       7.806   2.082 -18.526  1.00 24.66      A    C
ATOM    283  OD1 ASP A  39       6.796   1.945 -19.248  1.00 26.50      A    O
ATOM    284  OD2 ASP A  39       8.246   3.239 -18.372  1.00 27.03      A    O
ATOM    285  C   ASP A  39      10.480   2.075 -17.156  1.00 24.00      A    C
ATOM    286  O   ASP A  39      10.843   3.004 -16.434  1.00 23.68      A    O
ATOM    287  N   SER A  40      11.003   1.832 -18.355  1.00 24.67      A    N
ATOM    288  CA  SER A  40      12.166   2.539 -18.847  1.00 24.80      A    C
ATOM    289  CB  SER A  40      12.777   1.766 -20.041  1.00 25.30      A    C
ATOM    290  OG  SER A  40      11.925   1.881 -21.163  1.00 25.60      A    O
ATOM    291  C   SER A  40      11.815   3.984 -19.228  1.00 23.51      A    C
ATOM    292  O   SER A  40      12.687   4.805 -19.375  1.00 24.41      A    O
ATOM    293  N   SER A  41      10.532   4.308 -19.317  1.00 23.14      A    N
ATOM    294  CA  SER A  41      10.097   5.670 -19.621  1.00 21.75      A    C
ATOM    295  CB  SER A  41       8.620   5.679 -20.037  1.00 22.84      A    C
ATOM    296  OG  SER A  41       7.725   5.739 -18.919  1.00 21.43      A    O
ATOM    297  C   SER A  41      10.262   6.639 -18.427  1.00 21.13      A    C
ATOM    298  O   SER A  41      10.299   7.863 -18.603  1.00 19.88      A    O
ATOM    299  N   MET A  42      10.359   6.079 -17.223  1.00 19.68      A    N
ATOM    300  CA  MET A  42      10.381   6.882 -15.996  1.00 18.70      A    C
ATOM    301  CB  MET A  42      10.295   5.949 -14.782  1.00 18.20      A    C
ATOM    302  CG  MET A  42      10.451   6.626 -13.423  1.00 17.87      A    C
ATOM    303  SD  MET A  42       9.190   7.804 -13.030  1.00 16.31      A    S
ATOM    304  CE  MET A  42       7.658   6.844 -13.134  1.00 15.38      A    C
ATOM    305  C   MET A  42      11.607   7.779 -15.897  1.00 17.89      A    C
ATOM    306  O   MET A  42      12.728   7.390 -16.223  1.00 17.28      A    O
ATOM    307  N   HIS A  43      11.381   8.998 -15.421  1.00 17.69      A    N
ATOM    308  CA  HIS A  43      12.479   9.903 -15.081  1.00 17.38      A    C
ATOM    309  CB  HIS A  43      11.942  11.020 -14.196  1.00 17.29      A    C
ATOM    310  CG  HIS A  43      12.896  12.155 -13.981  1.00 16.73      A    C
ATOM    311  ND1 HIS A  43      12.576  13.456 -14.321  1.00 16.98      A    N
ATOM    312  CE1 HIS A  43      13.566  14.257 -13.971  1.00 13.61      A    C
ATOM    313  NE2 HIS A  43      14.521  13.523 -13.426  1.00 17.49      A    N
ATOM    314  CD2 HIS A  43      14.113  12.207 -13.397  1.00 13.70      A    C
ATOM    315  C   HIS A  43      13.647   9.209 -14.381  1.00 16.64      A    C
ATOM    316  O   HIS A  43      13.453   8.389 -13.479  1.00 15.82      A    O
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ATOM    317  N   GLU A  44      14.858   9.559 -14.818  1.00 16.35      A    N
ATOM    318  CA  GLU A  44      16.112   8.985 -14.358  1.00 16.74      A    C
ATOM    319  CB  GLU A  44      17.293   9.763 -14.988  1.00 17.71      A    C
ATOM    320  CG  GLU A  44      17.268  11.270 -14.753  1.00 18.20      A    C
ATOM    321  CD  GLU A  44      18.445  12.004 -15.418  1.00 22.20      A    C
ATOM    322  OE1 GLU A  44      18.997  11.455 -16.397  1.00 20.94      A    O
ATOM    323  OE2 GLU A  44      18.843  13.110 -14.933  1.00 20.93      A    O
ATOM    324  C   GLU A  44      16.280   8.982 -12.823  1.00 17.11      A    C
ATOM    325  O   GLU A  44      16.944   8.104 -12.259  1.00 17.08      A    O
ATOM    326  N   ALA A  45      15.665   9.954 -12.152  1.00 16.39      A    N
ATOM    327  CA  ALA A  45      15.774  10.061 -10.696  1.00 16.01      A    C
ATOM    328  CB  ALA A  45      15.122  11.354 -10.198  1.00 15.44      A    C
ATOM    329  C   ALA A  45      15.155   8.864  -9.971  1.00 16.39      A    C
ATOM    330  O   ALA A  45      15.538   8.564  -8.857  1.00 14.42      A    O
ATOM    331  N   PHE A  46      14.184   8.218 -10.595  1.00 16.01      A    N
ATOM    332  CA  PHE A  46      13.411   7.139  -9.971  1.00 16.28      A    C
ATOM    333  CB  PHE A  46      11.958   7.562  -9.882  1.00 16.14      A    C
ATOM    334  CG  PHE A  46      11.780   8.959  -9.396  1.00 14.90      A    C
ATOM    335  CD1 PHE A  46      12.036   9.275  -8.078  1.00 14.17      A    C
ATOM    336  CE1 PHE A  46      11.897  10.586  -7.628  1.00 13.19      A    C
ATOM    337  CZ  PHE A  46      11.525  11.592  -8.504  1.00 14.92      A    C
ATOM    338  CE2 PHE A  46      11.291  11.299  -9.809  1.00 16.01      A    C
ATOM    339  CD2 PHE A  46      11.416   9.971 -10.261  1.00 15.93      A    C
ATOM    340  C   PHE A  46      13.466   5.791 -10.697  1.00 17.23      A    C
ATOM    341  O   PHE A  46      13.017   4.764 -10.172  1.00 16.06      A    O
ATOM    342  N   ARG A  47      13.986   5.781 -11.917  1.00 18.87      A    N
ATOM    343  CA  ARG A  47      13.963   4.566 -12.723  1.00 20.32      A    C
ATOM    344  CB  ARG A  47      14.659   4.833 -14.062  1.00 21.00      A    C
ATOM    345  CG  ARG A  47      14.309   3.871 -15.173  1.00 24.13      A    C
ATOM    346  CD  ARG A  47      14.468   4.517 -16.570  1.00 28.53      A    C
ATOM    347  NE  ARG A  47      15.803   5.031 -16.813  1.00 32.22      A    N
ATOM    348  CZ  ARG A  47      16.105   6.229 -17.359  1.00 34.45      A    C
ATOM    349  NH1 ARG A  47      15.171   7.109 -17.703  1.00 33.97      A    N
ATOM    350  NH2 ARG A  47      17.384   6.558 -17.527  1.00 33.82      A    N
ATOM    351  C   ARG A  47      14.674   3.437 -12.000  1.00 20.49      A    C
ATOM    352  O   ARG A  47      15.784   3.619 -11.523  1.00 21.38      A    O
ATOM    353  N   GLY A  48      14.032   2.280 -11.898  1.00 21.45      A    N
ATOM    354  CA  GLY A  48      14.642   1.105 -11.274  1.00 21.59      A    C
ATOM    355  C   GLY A  48      14.583   1.091  -9.741  1.00 21.98      A    C
ATOM    356  O   GLY A  48      15.072   0.145  -9.102  1.00 21.74      A    O
ATOM    357  N   LYS A  49      13.984   2.117  -9.136  1.00 21.05      A    N
ATOM    358  CA  LYS A  49      13.950   2.197  -7.662  1.00 20.90      A    C
ATOM    359  CB  LYS A  49      14.915   3.305  -7.180  1.00 22.03      A    C
ATOM    360  CG  LYS A  49      14.366   4.713  -7.161  1.00 24.83      A    C
ATOM    361  CD  LYS A  49      15.447   5.815  -6.761  1.00 27.45      A    C
ATOM    362  CE  LYS A  49      15.957   5.680  -5.358  1.00 27.82      A    C
ATOM    363  NZ  LYS A  49      17.024   4.667  -5.220  1.00 28.25      A    N
ATOM    364  C   LYS A  49      12.523   2.329  -7.077  1.00 19.90      A    C
ATOM    365  O   LYS A  49      12.339   2.667  -5.890  1.00 19.91      A    O
ATOM    366  N   ILE A  50      11.523   1.999  -7.900  1.00 18.63      A    N
ATOM    367  CA  ILE A  50      10.121   2.078  -7.533  1.00 17.48      A    C
ATOM    368  CB  ILE A  50       9.284   2.650  -8.695  1.00 17.67      A    C
ATOM    369  CG1 ILE A  50       9.738   4.076  -9.050  1.00 17.24      A    C
ATOM    370  CD1 ILE A  50       9.083   4.630 -10.302  1.00 17.34      A    C
ATOM    371  CG2 ILE A  50       7.807   2.723  -8.319  1.00 17.29      A    C
ATOM    372  C   ILE A  50       9.562   0.730  -7.090  1.00 17.96      A    C
ATOM    373  O   ILE A  50       9.339  -0.161  -7.909  1.00 18.69      A    O
ATOM    374  N   THR A  51       9.355   0.583  -5.784  1.00 17.09      A    N
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ATOM    375  CA  THR A  51       8.731  -0.601  -5.218  1.00 17.60      A    C
ATOM    376  CB  THR A  51       8.700  -0.423  -3.690  1.00 18.38      A    C
ATOM    377  OG1 THR A  51      10.033  -0.380  -3.205  1.00 17.39      A    O
ATOM    378  CG2 THR A  51       8.054  -1.617  -3.014  1.00 17.34      A    C
ATOM    379  C   THR A  51       7.301  -0.746  -5.646  1.00 17.50      A    C
ATOM    380  O   THR A  51       6.827  -1.834  -5.903  1.00 18.10      A    O
ATOM    381  N   ALA A  52       6.578   0.369  -5.670  1.00 16.93      A    N
ATOM    382  CA  ALA A  52       5.179   0.338  -6.052  1.00 17.34      A    C
ATOM    383  CB  ALA A  52       4.314  -0.132  -4.884  1.00 17.41      A    C
ATOM    384  C   ALA A  52       4.753   1.725  -6.501  1.00 17.46      A    C
ATOM    385  O   ALA A  52       5.187   2.730  -5.928  1.00 16.50      A    O
ATOM    386  N   LEU A  53       3.921   1.760  -7.539  1.00 17.19      A    N
ATOM    387  CA  LEU A  53       3.369   2.987  -8.081  1.00 16.89      A    C
ATOM    388  CB  LEU A  53       4.004   3.309  -9.430  1.00 16.66      A    C
ATOM    389  CG  LEU A  53       3.490   4.525 -10.224  1.00 16.83      A    C
ATOM    390  CD1 LEU A  53       3.523   5.796  -9.401  1.00 15.83      A    C
ATOM    391  CD2 LEU A  53       4.303   4.720 -11.476  1.00 17.71      A    C
ATOM    392  C   LEU A  53       1.868   2.779  -8.212  1.00 17.28      A    C
ATOM    393  O   LEU A  53       1.421   2.057  -9.097  1.00 17.43      A    O
ATOM    394  N   TYR A  54       1.101   3.393  -7.303  1.00 17.28      A    N
ATOM    395  CA  TYR A  54      -0.350   3.200  -7.230  1.00 16.87      A    C
ATOM    396  CB  TYR A  54      -0.774   2.944  -5.789  1.00 16.88      A    C
ATOM    397  CG  TYR A  54      -0.268   1.679  -5.144  1.00 15.63      A    C
ATOM    398  CD1 TYR A  54      -0.411   0.448  -5.770  1.00 15.86      A    C
ATOM    399  CE1 TYR A  54       0.037  -0.698  -5.192  1.00 15.12      A    C
ATOM    400  CZ  TYR A  54       0.666  -0.647  -3.946  1.00 15.32      A    C
ATOM    401  OH  TYR A  54       1.093  -1.815  -3.374  1.00 14.97      A    O
ATOM    402  CE2 TYR A  54       0.856   0.558  -3.312  1.00 15.70      A    C
ATOM    403  CD2 TYR A  54       0.384   1.718  -3.908  1.00 15.59      A    C
ATOM    404  C   TYR A  54      -1.098   4.411  -7.712  1.00 17.11      A    C
ATOM    405  O   TYR A  54      -0.733   5.546  -7.387  1.00 16.78      A    O
ATOM    406  N   ALA A  55      -2.161   4.184  -8.483  1.00 17.01      A    N
ATOM    407  CA  ALA A  55      -3.032   5.260  -8.926  1.00 17.49      A    C
ATOM    408  CB  ALA A  55      -3.355   5.094 -10.437  1.00 17.43      A    C
ATOM    409  C   ALA A  55      -4.323   5.272  -8.100  1.00 18.26      A    C
ATOM    410  O   ALA A  55      -5.174   4.400  -8.269  1.00 19.60      A    O
ATOM    411  N   LEU A  56      -4.481   6.267  -7.230  1.00 17.69      A    N
ATOM    412  CA  LEU A  56      -5.641   6.353  -6.368  1.00 17.32      A    C
ATOM    413  CB  LEU A  56      -5.224   6.779  -4.965  1.00 16.99      A    C
ATOM    414  CG  LEU A  56      -4.452   5.752  -4.129  1.00 17.97      A    C
ATOM    415  CD1 LEU A  56      -3.120   5.532  -4.719  1.00 20.33      A    C
ATOM    416  CD2 LEU A  56      -4.329   6.225  -2.662  1.00 19.18      A    C
ATOM    417  C   LEU A  56      -6.662   7.360  -6.867  1.00 17.28      A    C
ATOM    418  O   LEU A  56      -7.839   7.192  -6.653  1.00 17.95      A    O
ATOM    419  N   GLY A  57      -6.204   8.430  -7.485  1.00 17.26      A    N
ATOM    420  CA  GLY A  57      -7.068   9.541  -7.802  1.00 17.53      A    C
ATOM    421  C   GLY A  57      -7.662   9.430  -9.199  1.00 17.74      A    C
ATOM    422  O   GLY A  57      -8.758   9.905  -9.446  1.00 17.69      A    O
ATOM    423  N   ARG A  58      -6.921   8.825 -10.109  1.00 18.54      A    N
ATOM    424  CA  ARG A  58      -7.361   8.659 -11.502  1.00 19.44      A    C
ATOM    425  CB  ARG A  58      -6.572   9.555 -12.466  1.00 18.56      A    C
ATOM    426  CG  ARG A  58      -6.873  11.036 -12.371  1.00 18.16      A    C
ATOM    427  CD  ARG A  58      -5.685  11.912 -12.787  1.00 17.99      A    C
ATOM    428  NE  ARG A  58      -4.505  11.593 -11.990  1.00 17.16      A    N
ATOM    429  CZ  ARG A  58      -3.248  11.716 -12.392  1.00 18.78      A    C
ATOM    430  NH1 ARG A  58      -2.967  12.194 -13.591  1.00 18.96      A    N
ATOM    431  NH2 ARG A  58      -2.253  11.339 -11.584  1.00 17.60      A    N
ATOM    432  C   ARG A  58      -7.123   7.240 -11.909  1.00 19.97      A    C
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ATOM    433  O   ARG A  58      -6.007   6.754 -11.878  1.00 20.06      A    O
ATOM    434  N   THR A  59      -8.183   6.575 -12.324  1.00 22.06      A    N
ATOM    435  CA  THR A  59      -8.091   5.180 -12.688  1.00 22.88      A    C
ATOM    436  CB  THR A  59      -9.479   4.693 -13.142  1.00 24.04      A    C
ATOM    437  OG1 THR A  59     -10.330   4.643 -11.984  1.00 25.24      A    O
ATOM    438  CG2 THR A  59      -9.406   3.250 -13.657  1.00 25.24      A    C
ATOM    439  C   THR A  59      -7.009   4.919 -13.733  1.00 22.06      A    C
ATOM    440  O   THR A  59      -7.020   5.482 -14.835  1.00 22.93      A    O
ATOM    441  N   ASN A  60      -6.074   4.068 -13.332  1.00 21.27      A    N
ATOM    442  CA  ASN A  60      -4.939   3.618 -14.124  1.00 21.57      A    C
ATOM    443  CB  ASN A  60      -5.400   2.788 -15.326  1.00 22.51      A    C
ATOM    444  CG  ASN A  60      -5.861   1.401 -14.927  1.00 24.76      A    C
ATOM    445  OD1 ASN A  60      -5.546   0.908 -13.835  1.00 27.82      A    O
ATOM    446  ND2 ASN A  60      -6.624   0.773 -15.801  1.00 25.97      A    N
ATOM    447  C   ASN A  60      -4.038   4.744 -14.614  1.00 20.35      A    C
ATOM    448  O   ASN A  60      -3.369   4.589 -15.629  1.00 20.71      A    O
ATOM    449  N   ASN A  61      -4.023   5.852 -13.897  1.00 18.43      A    N
ATOM    450  CA  ASN A  61      -3.217   6.996 -14.300  1.00 18.53      A    C
ATOM    451  CB  ASN A  61      -4.095   8.062 -14.972  1.00 17.54      A    C
ATOM    452  CG  ASN A  61      -3.278   9.194 -15.580  1.00 19.62      A    C
ATOM    453  OD1 ASN A  61      -3.832  10.171 -16.141  1.00 22.44      A    O
ATOM    454  ND2 ASN A  61      -1.968   9.081 -15.481  1.00 15.52      A    N
ATOM    455  C   ASN A  61      -2.520   7.586 -13.088  1.00 16.75      A    C
ATOM    456  O   ASN A  61      -3.159   8.213 -12.260  1.00 16.00      A    O
ATOM    457  N   ALA A  62      -1.219   7.357 -12.988  1.00 16.29      A    N
ATOM    458  CA  ALA A  62      -0.418   7.910 -11.902  1.00 16.34      A    C
ATOM    459  CB  ALA A  62       0.310   6.804 -11.183  1.00 16.55      A    C
ATOM    460  C   ALA A  62       0.584   8.948 -12.405  1.00 16.52      A    C
ATOM    461  O   ALA A  62       1.583   9.221 -11.728  1.00 15.61      A    O
ATOM    462  N   ASN A  63       0.344   9.515 -13.593  1.00 15.91      A    N
ATOM    463  CA  ASN A  63       1.276  10.465 -14.157  1.00 15.75      A    C
ATOM    464  CB  ASN A  63       1.251  10.471 -15.720  1.00 15.36      A    C
ATOM    465  CG  ASN A  63       0.043  11.165 -16.307  1.00 16.00      A    C
ATOM    466  OD1 ASN A  63      -0.617  11.982 -15.643  1.00 14.50      A    O
ATOM    467  ND2 ASN A  63      -0.274  10.833 -17.584  1.00 15.36      A    N
ATOM    468  C   ASN A  63       1.115  11.858 -13.518  1.00 15.21      A    C
ATOM    469  O   ASN A  63       0.168  12.108 -12.762  1.00 15.63      A    O
ATOM    470  N   ASP A  64       2.047  12.753 -13.828  1.00 15.12      A    N
ATOM    471  CA  ASP A  64       2.192  14.015 -13.102  1.00 15.29      A    C
ATOM    472  CB  ASP A  64       3.450  13.990 -12.233  1.00 14.59      A    C
ATOM    473  CG  ASP A  64       3.532  15.161 -11.300  1.00 15.31      A    C
ATOM    474  OD1 ASP A  64       2.476  15.813 -11.058  1.00 14.15      A    O
ATOM    475  OD2 ASP A  64       4.626  15.516 -10.776  1.00 14.37      A    O
ATOM    476  C   ASP A  64       2.236  15.206 -14.061  1.00 15.53      A    C
ATOM    477  O   ASP A  64       3.315  15.713 -14.423  1.00 16.54      A    O
ATOM    478  N   PRO A  65       1.065  15.644 -14.476  1.00 16.18      A    N
ATOM    479  CA  PRO A  65       0.950  16.813 -15.343  1.00 17.33      A    C
ATOM    480  CB  PRO A  65      -0.509  16.776 -15.807  1.00 17.19      A    C
ATOM    481  CG  PRO A  65      -1.225  15.953 -14.808  1.00 17.73      A    C
ATOM    482  CD  PRO A  65      -0.249  15.043 -14.172  1.00 17.21      A    C
ATOM    483  C   PRO A  65       1.228  18.102 -14.607  1.00 17.72      A    C
ATOM    484  O   PRO A  65       1.515  19.081 -15.250  1.00 17.98      A    O
ATOM    485  N   ASN A  66       1.150  18.065 -13.279  1.00 18.27      A    N
ATOM    486  CA  ASN A  66       1.314  19.217 -12.426  1.00 19.24      A    C
ATOM    487  CB  ASN A  66       0.536  18.958 -11.111  1.00 20.48      A    C
ATOM    488  CG  ASN A  66       0.790  19.993 -10.068  1.00 22.89      A    C
ATOM    489  OD1 ASN A  66       1.942  20.281  -9.721  1.00 23.54      A    O
ATOM    490  ND2 ASN A  66      -0.287  20.591  -9.566  1.00 25.20      A    N
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ATOM    491  C    ASN A  66       2.806  19.457 -12.153  1.00 18.71      A    C
ATOM    492  O    ASN A  66       3.314  20.549 -12.353  1.00 18.84      A    O
ATOM    493  N    GLY A  67       3.500  18.426 -11.698  1.00 17.55      A    N
ATOM    494  CA   GLY A  67       4.917  18.503 -11.406  1.00 16.38      A    C
ATOM    495  C    GLY A  67       5.234  18.455  -9.916  1.00 15.32      A    C
ATOM    496  O    GLY A  67       6.383  18.167  -9.542  1.00 15.11      A    O
ATOM    497  N    HIS A  68       4.230  18.722  -9.075  1.00 13.44      A    N
ATOM    498  CA   HIS A  68       4.406  18.776  -7.608  1.00 12.51      A    C
ATOM    499  CB BHIS A  68       3.109  19.121  -6.891  0.50 12.22      A    C
ATOM    500  CB AHIS A  68       3.048  19.078  -6.930  0.50 12.48      A    C
ATOM    501  CG BHIS A  68       3.266  19.371  -5.417  0.50 10.61      A    C
ATOM    502  CG AHIS A  68       3.140  19.398  -5.464  0.50 10.86      A    C
ATOM    503  ND1BHIS A  68       2.741  18.522  -4.453  0.50  5.34      A    N
ATOM    504  ND1AHIS A  68       3.742  18.559  -4.548  0.50  7.56      A    N
ATOM    505  CE1BHIS A  68       3.009  19.016  -3.254  0.50  6.59      A    C
ATOM    506  CE1AHIS A  68       3.674  19.102  -3.341  0.50  2.00      A    C
ATOM    507  NE2BHIS A  68       3.678  20.158  -3.403  0.50  7.98      A    N
ATOM    508  NE2AHIS A  68       3.061  20.277  -3.442  0.50  6.21      A    N
ATOM    509  CD2BHIS A  68       3.845  20.405  -4.745  0.50  5.10      A    C
ATOM    510  CD2AHIS A  68       2.697  20.471  -4.756  0.50  8.79      A    C
ATOM    511  C    HIS A  68       4.986  17.474  -7.064  1.00 12.70      A    C
ATOM    512  O    HIS A  68       6.025  17.471  -6.401  1.00 12.91      A    O
ATOM    513  N    GLY A  69       4.315  16.374  -7.317  1.00 13.22      A    N
ATOM    514  CA   GLY A  69       4.709  15.094  -6.739  1.00 13.52      A    C
ATOM    515  C    GLY A  69       6.039  14.574  -7.181  1.00 13.01      A    C
ATOM    516  O    GLY A  69       6.751  13.894  -6.418  1.00 13.80      A    O
ATOM    517  N    THR A  70       6.391  14.865  -8.432  1.00 13.25      A    N
ATOM    518  CA   THR A  70       7.651  14.425  -8.970  1.00 12.89      A    C
ATOM    519  CB   THR A  70       7.688  14.638 -10.507  1.00 13.93      A    C
ATOM    520  OG1  THR A  70       6.592  13.940 -11.116  1.00 14.34      A    O
ATOM    521  CG2  THR A  70       8.895  13.977 -11.110  1.00 13.50      A    C
ATOM    522  C    THR A  70       8.769  15.192  -8.309  1.00 12.86      A    C
ATOM    523  O    THR A  70       9.816  14.622  -8.013  1.00 13.63      A    O
ATOM    524  N    HIS A  71       8.560  16.498  -8.093  1.00 12.19      A    N
ATOM    525  CA   HIS A  71       9.580  17.341  -7.486  1.00 11.80      A    C
ATOM    526  CB   HIS A  71       9.125  18.796  -7.555  1.00 11.41      A    C
ATOM    527  CG BHIS A  71      10.185  19.784  -7.212  0.50 11.89      A    C
ATOM    528  CG AHIS A  71      10.189  19.775  -7.181  0.50  9.73      A    C
ATOM    529  ND1BHIS A  71      10.926  19.709  -6.050  0.50 12.60      A    N
ATOM    530  ND1AHIS A  71      10.236  20.388  -5.942  0.50  5.89      A    N
ATOM    531  CE1BHIS A  71      11.791  20.706  -6.025  0.50 13.16      A    C
ATOM    532  CE1AHIS A  71      11.281  21.192  -5.898  0.50  7.95      A    C
ATOM    533  NE2BHIS A  71      11.618  21.438  -7.114  0.50 14.18      A    N
ATOM    534  NE2AHIS A  71      11.923  21.107  -7.054  0.50 10.14      A    N
ATOM    535  CD2BHIS A  71      10.617  20.883  -7.869  0.50 10.25      A    C
ATOM    536  CD2AHIS A  71      11.258  20.231  -7.874  0.50  6.22      A    C
ATOM    537  C    HIS A  71       9.806  16.875  -6.018  1.00 12.35      A    C
ATOM    538  O    HIS A  71      10.935  16.698  -5.538  1.00 12.45      A    O
ATOM    539  N    VAL A  72       8.697  16.657  -5.331  1.00 12.33      A    N
ATOM    540  CA   VAL A  72       8.704  16.204  -3.960  1.00 12.62      A    C
ATOM    541  CB   VAL A  72       7.279  16.056  -3.469  1.00 12.75      A    C
ATOM    542  CG1  VAL A  72       7.248  15.256  -2.202  1.00 12.50      A    C
ATOM    543  CG2  VAL A  72       6.647  17.430  -3.262  1.00 12.97      A    C
ATOM    544  C    VAL A  72       9.431  14.864  -3.799  1.00 13.01      A    C
ATOM    545  O    VAL A  72      10.333  14.707  -2.947  1.00 12.02      A    O
ATOM    546  N    ALA A  73       9.054  13.888  -4.615  1.00 12.23      A    N
ATOM    547  CA   ALA A  73       9.664  12.572  -4.521  1.00 12.29      A    C
ATOM    548  CB   ALA A  73       8.986  11.617  -5.440  1.00 12.32      A    C
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ATOM	549	C	ALA	A	73	11.180	12.682	-4.850	1.00	11.78	A	C
ATOM	550	O	ALA	A	73	11.985	11.992	-4.280	1.00	11.60	A	O
ATOM	551	N	GLY	A	74	11.553	13.583	-5.742	1.00	12.04	A	N
ATOM	552	CA	GLY	A	74	12.961	13.760	-6.069	1.00	11.92	A	C
ATOM	553	C	GLY	A	74	13.768	14.190	-4.845	1.00	12.13	A	C
ATOM	554	O	GLY	A	74	14.936	13.816	-4.693	1.00	11.64	A	O
ATOM	555	N	SER	A	75	13.157	15.015	-3.994	1.00	12.08	A	N
ATOM	556	CA	SER	A	75	13.844	15.546	-2.827	1.00	12.08	A	C
ATOM	557	CB	SER	A	75	13.095	16.748	-2.267	1.00	11.53	A	C
ATOM	558	OG	SER	A	75	13.254	17.915	-3.077	1.00	13.29	A	O
ATOM	559	C	SER	A	75	14.033	14.477	-1.739	1.00	12.05	A	C
ATOM	560	O	SER	A	75	14.984	14.540	-0.927	1.00	12.73	A	O
ATOM	561	N	VAL	A	76	13.112	13.524	-1.676	1.00	11.61	A	N
ATOM	562	CA	VAL	A	76	13.272	12.407	-0.748	1.00	11.87	A	C
ATOM	563	CB	VAL	A	76	12.023	11.519	-0.691	1.00	12.06	A	C
ATOM	564	CG1	VAL	A	76	12.224	10.396	0.324	1.00	12.75	A	C
ATOM	565	CG2	VAL	A	76	10.799	12.319	-0.316	1.00	11.56	A	C
ATOM	566	C	VAL	A	76	14.415	11.501	-1.173	1.00	12.11	A	C
ATOM	567	O	VAL	A	76	15.280	11.158	-0.372	1.00	10.37	A	O
ATOM	568	N	LEU	A	77	14.410	11.085	-2.437	1.00	12.79	A	N
ATOM	569	CA	LEU	A	77	15.234	9.934	-2.809	1.00	12.61	A	C
ATOM	570	CB	LEU	A	77	14.532	8.627	-2.425	1.00	13.05	A	C
ATOM	571	CG	LEU	A	77	13.050	8.419	-2.774	1.00	11.85	A	C
ATOM	572	CD1	LEU	A	77	12.868	8.361	-4.281	1.00	12.80	A	C
ATOM	573	CD2	LEU	A	77	12.512	7.140	-2.114	1.00	14.07	A	C
ATOM	574	C	LEU	A	77	15.676	9.847	-4.267	1.00	13.21	A	C
ATOM	575	O	LEU	A	77	16.181	8.810	-4.656	1.00	13.59	A	O
ATOM	576	N	GLY	A	78	15.586	10.935	-5.022	1.00	13.72	A	N
ATOM	577	CA	GLY	A	78	16.045	10.945	-6.415	1.00	14.19	A	C
ATOM	578	C	GLY	A	78	17.486	10.505	-6.506	1.00	14.88	A	C
ATOM	579	O	GLY	A	78	18.322	10.998	-5.718	1.00	14.70	A	O
ATOM	580	N	ASN	A	79	17.800	9.587	-7.420	1.00	15.24	A	N
ATOM	581	CA	ASN	A	79	19.172	9.066	-7.520	1.00	16.71	A	C
ATOM	582	CB	ASN	A	79	19.204	7.542	-7.263	1.00	16.08	A	C
ATOM	583	CG	ASN	A	79	20.615	7.023	-6.904	1.00	16.70	A	C
ATOM	584	OD1	ASN	A	79	21.438	7.754	-6.372	1.00	15.21	A	O
ATOM	585	ND2	ASN	A	79	20.881	5.749	-7.181	1.00	15.92	A	N
ATOM	586	C	ASN	A	79	19.877	9.353	-8.852	1.00	18.12	A	C
ATOM	587	O	ASN	A	79	20.735	8.576	-9.267	1.00	18.96	A	O
ATOM	588	N	ALA	A	80	19.559	10.458	-9.513	1.00	18.68	A	N
ATOM	589	CA	ALA	A	80	20.316	10.838	-10.723	1.00	19.08	A	C
ATOM	590	CB	ALA	A	80	19.381	11.169	-11.876	1.00	19.15	A	C
ATOM	591	C	ALA	A	80	21.261	11.995	-10.376	1.00	18.85	A	C
ATOM	592	O	ALA	A	80	22.245	11.795	-9.663	1.00	18.76	A	O
ATOM	593	N	THR	A	81	20.973	13.194	-10.841	1.00	18.39	A	N
ATOM	594	CA	THR	A	81	21.647	14.370	-10.305	1.00	18.18	A	C
ATOM	595	CB	THR	A	81	22.229	15.222	-11.444	1.00	18.72	A	C
ATOM	596	OG1	THR	A	81	21.202	15.535	-12.379	1.00	17.48	A	O
ATOM	597	CG2	THR	A	81	23.229	14.420	-12.289	1.00	21.52	A	C
ATOM	598	C	THR	A	81	20.650	15.185	-9.470	1.00	17.64	A	C
ATOM	599	O	THR	A	81	19.466	14.858	-9.423	1.00	17.77	A	O
ATOM	600	N	ASN	A	82	21.115	16.238	-8.803	1.00	16.86	A	N
ATOM	601	CA	ASN	A	82	20.271	16.947	-7.842	1.00	16.82	A	C
ATOM	602	CB	ASN	A	82	19.279	17.840	-8.574	1.00	16.90	A	C
ATOM	603	CG	ASN	A	82	19.962	18.782	-9.552	1.00	18.05	A	C
ATOM	604	OD1	ASN	A	82	19.861	18.632	-10.804	1.00	20.14	A	O
ATOM	605	ND2	ASN	A	82	20.650	19.760	-9.005	1.00	12.31	A	N
ATOM	606	C	ASN	A	82	19.541	15.941	-6.930	1.00	16.16	A	C

ATOM	607	O	ASN	A	82	18.325	15.985	-6.772	1.00	16.88	A	O
ATOM	608	N	LYS	A	83	20.310	15.022	-6.366	1.00	15.41	A	N
ATOM	609	CA	LYS	A	83	19.767	13.853	-5.710	1.00	15.60	A	C
ATOM	610	CB	LYS	A	83	20.907	12.919	-5.287	1.00	15.95	A	C
ATOM	611	CG	LYS	A	83	21.665	12.168	-6.415	1.00	16.19	A	C
ATOM	612	CD	LYS	A	83	22.815	11.339	-5.811	1.00	19.24	A	C
ATOM	613	CE	LYS	A	83	23.806	10.791	-6.833	1.00	21.12	A	C
ATOM	614	NZ	LYS	A	83	23.076	9.941	-7.791	1.00	20.88	A	N
ATOM	615	C	LYS	A	83	18.966	14.243	-4.453	1.00	14.74	A	C
ATOM	616	O	LYS	A	83	19.243	15.248	-3.801	1.00	13.71	A	O
ATOM	617	N	GLY	A	84	18.000	13.402	-4.117	1.00	14.66	A	N
ATOM	618	CA	GLY	A	84	17.337	13.439	-2.833	1.00	14.40	A	C
ATOM	619	C	GLY	A	84	18.240	13.078	-1.664	1.00	14.38	A	C
ATOM	620	O	GLY	A	84	19.372	12.683	-1.853	1.00	14.68	A	O
ATOM	621	N	MET	A	85	17.734	13.231	-0.439	1.00	13.41	A	N
ATOM	622	CA	MET	A	85	18.586	13.079	0.753	1.00	13.39	A	C
ATOM	623	CB	MET	A	85	17.865	13.660	1.970	1.00	13.62	A	C
ATOM	624	CG	MET	A	85	17.446	15.132	1.799	1.00	14.10	A	C
ATOM	625	SD	MET	A	85	18.823	16.235	1.480	1.00	15.77	A	S
ATOM	626	CE	MET	A	85	18.801	16.373	-0.341	1.00	16.54	A	C
ATOM	627	C	MET	A	85	18.946	11.600	1.022	1.00	13.55	A	C
ATOM	628	O	MET	A	85	19.975	11.302	1.623	1.00	13.91	A	O
ATOM	629	N	ALA	A	86	18.078	10.685	0.586	1.00	13.51	A	N
ATOM	630	CA	ALA	A	86	18.290	9.250	0.774	1.00	13.69	A	C
ATOM	631	CB	ALA	A	86	17.223	8.682	1.717	1.00	13.63	A	C
ATOM	632	C	ALA	A	86	18.200	8.571	-0.589	1.00	13.59	A	C
ATOM	633	O	ALA	A	86	17.258	7.821	-0.868	1.00	14.50	A	O
ATOM	634	N	PRO	A	87	19.175	8.818	-1.445	1.00	14.33	A	N
ATOM	635	CA	PRO	A	87	19.068	8.409	-2.859	1.00	14.18	A	C
ATOM	636	CB	PRO	A	87	20.236	9.152	-3.515	1.00	14.93	A	C
ATOM	637	CG	PRO	A	87	21.263	9.267	-2.393	1.00	14.56	A	C
ATOM	638	CD	PRO	A	87	20.446	9.524	-1.148	1.00	13.97	A	C
ATOM	639	C	PRO	A	87	19.146	6.901	-3.123	1.00	14.68	A	C
ATOM	640	O	PRO	A	87	18.943	6.474	-4.260	1.00	15.65	A	O
ATOM	641	N	GLN	A	88	19.424	6.099	-2.109	1.00	15.11	A	N
ATOM	642	CA	GLN	A	88	19.436	4.639	-2.266	1.00	16.35	A	C
ATOM	643	CB	GLN	A	88	20.748	4.050	-1.733	1.00	16.73	A	C
ATOM	644	CG	GLN	A	88	21.900	4.262	-2.703	1.00	19.50	A	C
ATOM	645	CD	GLN	A	88	23.267	3.916	-2.161	1.00	21.39	A	C
ATOM	646	OE1	GLN	A	88	23.427	2.933	-1.439	1.00	22.79	A	O
ATOM	647	NE2	GLN	A	88	24.272	4.709	-2.547	1.00	22.41	A	N
ATOM	648	C	GLN	A	88	18.228	3.976	-1.621	1.00	16.49	A	C
ATOM	649	O	GLN	A	88	18.080	2.754	-1.644	1.00	16.50	A	O
ATOM	650	N	ALA	A	89	17.347	4.786	-1.044	1.00	16.72	A	N
ATOM	651	CA	ALA	A	89	16.056	4.279	-0.599	1.00	16.78	A	C
ATOM	652	CB	ALA	A	89	15.380	5.277	0.375	1.00	17.28	A	C
ATOM	653	C	ALA	A	89	15.139	3.996	-1.792	1.00	16.32	A	C
ATOM	654	O	ALA	A	89	15.212	4.648	-2.826	1.00	16.81	A	O
ATOM	655	N	ASN	A	90	14.248	3.037	-1.634	1.00	15.45	A	N
ATOM	656	CA	ASN	A	90	13.264	2.756	-2.658	1.00	15.40	A	C
ATOM	657	CB	ASN	A	90	13.036	1.247	-2.756	1.00	16.05	A	C
ATOM	658	CG	ASN	A	90	14.076	0.549	-3.658	1.00	19.92	A	C
ATOM	659	OD1	ASN	A	90	15.039	1.155	-4.106	1.00	25.00	A	O
ATOM	660	ND2	ASN	A	90	13.892	-0.736	-3.873	1.00	28.28	A	N
ATOM	661	C	ASN	A	90	11.942	3.486	-2.367	1.00	14.01	A	C
ATOM	662	O	ASN	A	90	11.668	3.834	-1.234	1.00	12.81	A	O
ATOM	663	N	LEU	A	91	11.150	3.705	-3.410	1.00	13.02	A	N
ATOM	664	CA	LEU	A	91	9.964	4.542	-3.381	1.00	13.78	A	C

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ATOM    665  CB  LEU A  91      10.022   5.524  -4.540  1.00 13.95      A    C
ATOM    666  CG  LEU A  91       8.861   6.472  -4.765  1.00 12.85      A    C
ATOM    667  CD1 LEU A  91       8.669   7.375  -3.571  1.00 15.80      A    C
ATOM    668  CD2 LEU A  91       9.077   7.287  -6.026  1.00 13.13      A    C
ATOM    669  C   LEU A  91       8.661   3.762  -3.524  1.00 14.15      A    C
ATOM    670  O   LEU A  91       8.503   2.953  -4.437  1.00 15.63      A    O
ATOM    671  N   VAL A  92       7.716   4.055  -2.649  1.00 13.69      A    N
ATOM    672  CA  VAL A  92       6.327   3.692  -2.872  1.00 14.00      A    C
ATOM    673  CB  VAL A  92       5.737   3.031  -1.662  1.00 13.15      A    C
ATOM    674  CG1 VAL A  92       4.197   3.018  -1.767  1.00 15.32      A    C
ATOM    675  CG2 VAL A  92       6.260   1.621  -1.546  1.00 13.02      A    C
ATOM    676  C   VAL A  92       5.615   5.001  -3.175  1.00 13.45      A    C
ATOM    677  O   VAL A  92       5.687   5.942  -2.376  1.00 13.53      A    O
ATOM    678  N   PHE A  93       4.984   5.107  -4.346  1.00 13.19      A    N
ATOM    679  CA  PHE A  93       4.293   6.351  -4.714  1.00 13.05      A    C
ATOM    680  CB  PHE A  93       4.899   6.964  -5.985  1.00 13.57      A    C
ATOM    681  CG  PHE A  93       4.484   8.388  -6.206  1.00 13.50      A    C
ATOM    682  CD1 PHE A  93       5.331   9.439  -5.861  1.00 13.00      A    C
ATOM    683  CE1 PHE A  93       4.941  10.748  -6.023  1.00 12.71      A    C
ATOM    684  CZ  PHE A  93       3.680  11.030  -6.515  1.00 11.77      A    C
ATOM    685  CE2 PHE A  93       2.832   9.998  -6.881  1.00 12.22      A    C
ATOM    686  CD2 PHE A  93       3.226   8.679  -6.710  1.00 12.44      A    C
ATOM    687  C   PHE A  93       2.793   6.150  -4.872  1.00 13.51      A    C
ATOM    688  O   PHE A  93       2.350   5.285  -5.632  1.00 13.61      A    O
ATOM    689  N   GLN A  94       2.021   6.949  -4.150  1.00 13.35      A    N
ATOM    690  CA  GLN A  94       0.567   6.903  -4.197  1.00 13.55      A    C
ATOM    691  CB  GLN A  94      -0.034   6.775  -2.786  1.00 12.95      A    C
ATOM    692  CG  GLN A  94       0.383   5.493  -2.078  1.00 13.25      A    C
ATOM    693  CD  GLN A  94       0.065   5.494  -0.589  1.00 14.07      A    C
ATOM    694  OE1 GLN A  94       0.598   6.311   0.157  1.00 16.83      A    O
ATOM    695  NE2 GLN A  94      -0.813   4.578  -0.158  1.00 13.83      A    N
ATOM    696  C   GLN A  94       0.118   8.195  -4.841  1.00 13.81      A    C
ATOM    697  O   GLN A  94       0.197   9.289  -4.236  1.00 12.11      A    O
ATOM    698  N   SER A  95      -0.266   8.072  -6.110  1.00 14.33      A    N
ATOM    699  CA  SER A  95      -0.793   9.190  -6.893  1.00 14.08      A    C
ATOM    700  CB  SER A  95      -0.743   8.850  -8.380  1.00 13.95      A    C
ATOM    701  OG  SER A  95      -1.337   9.864  -9.152  1.00 11.92      A    O
ATOM    702  C   SER A  95      -2.221   9.519  -6.494  1.00 14.82      A    C
ATOM    703  O   SER A  95      -3.150   8.743  -6.780  1.00 14.73      A    O
ATOM    704  N   ILE A  96      -2.404  10.681  -5.852  1.00 15.21      A    N
ATOM    705  CA  ILE A  96      -3.699  11.049  -5.277  1.00 15.55      A    C
ATOM    706  CB  ILE A  96      -3.560  11.482  -3.782  1.00 15.92      A    C
ATOM    707  CG1 ILE A  96      -2.466  12.548  -3.597  1.00 16.08      A    C
ATOM    708  CD1 ILE A  96      -2.367  13.122  -2.196  1.00 17.02      A    C
ATOM    709  CG2 ILE A  96      -3.257  10.273  -2.915  1.00 16.70      A    C
ATOM    710  C   ILE A  96      -4.398  12.158  -6.043  1.00 15.93      A    C
ATOM    711  O   ILE A  96      -5.475  12.590  -5.660  1.00 14.84      A    O
ATOM    712  N   MET A  97      -3.797  12.640  -7.119  1.00 16.32      A    N
ATOM    713  CA  MET A  97      -4.440  13.700  -7.889  1.00 18.17      A    C
ATOM    714  CB  MET A  97      -3.471  14.346  -8.884  1.00 18.20      A    C
ATOM    715  CG  MET A  97      -4.107  15.480  -9.688  1.00 21.58      A    C
ATOM    716  SD  MET A  97      -2.949  16.297 -10.814  1.00 25.41      A    S
ATOM    717  CE  MET A  97      -3.900  16.196 -12.225  1.00 31.75      A    C
ATOM    718  C   MET A  97      -5.647  13.114  -8.641  1.00 18.32      A    C
ATOM    719  O   MET A  97      -5.537  12.054  -9.249  1.00 18.26      A    O
ATOM    720  N   ASP A  98      -6.780  13.807  -8.568  1.00 19.35      A    N
ATOM    721  CA  ASP A  98      -8.020  13.369  -9.217  1.00 20.45      A    C
ATOM    722  CB  ASP A  98      -9.268  13.714  -8.375  1.00 20.39      A    C
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ATOM    723  CG  ASP A  98      -9.367  15.170  -8.021  1.00 21.41      A    C
ATOM    724  OD1 ASP A  98      -9.234  16.024  -8.928  1.00 22.52      A    O
ATOM    725  OD2 ASP A  98      -9.599  15.575  -6.847  1.00 20.32      A    O
ATOM    726  C   ASP A  98      -8.093  14.004 -10.592  1.00 20.49      A    C
ATOM    727  O   ASP A  98      -7.168  14.690 -10.996  1.00 19.61      A    O
ATOM    728  N   SER A  99      -9.170  13.747 -11.321  1.00 21.70      A    N
ATOM    729  CA  SER A  99      -9.252  14.202 -12.703  1.00 23.74      A    C
ATOM    730  CB  SER A  99     -10.202  13.301 -13.510  1.00 24.07      A    C
ATOM    731  OG  SER A  99     -11.497  13.436 -12.986  1.00 25.19      A    O
ATOM    732  C   SER A  99      -9.727  15.660 -12.749  1.00 24.80      A    C
ATOM    733  O   SER A  99      -9.696  16.286 -13.812  1.00 27.46      A    O
ATOM    734  N   GLY A 100     -10.152  16.203 -11.611  1.00 24.38      A    N
ATOM    735  CA  GLY A 100     -10.425  17.621 -11.488  1.00 25.17      A    C
ATOM    736  C   GLY A 100      -9.262  18.470 -10.968  1.00 25.36      A    C
ATOM    737  O   GLY A 100      -9.475  19.606 -10.557  1.00 26.29      A    O
ATOM    738  N   GLY A 101      -8.047  17.933 -10.964  1.00 25.13      A    N
ATOM    739  CA  GLY A 101      -6.873  18.715 -10.573  1.00 24.90      A    C
ATOM    740  C   GLY A 101      -6.541  18.760  -9.076  1.00 24.55      A    C
ATOM    741  O   GLY A 101      -5.425  19.133  -8.713  1.00 26.15      A    O
ATOM    742  N   GLY A 102      -7.490  18.406  -8.221  1.00 22.32      A    N
ATOM    743  CA  GLY A 102      -7.258  18.339  -6.783  1.00 21.84      A    C
ATOM    744  C   GLY A 102      -6.703  17.008  -6.267  1.00 20.73      A    C
ATOM    745  O   GLY A 102      -6.172  16.204  -7.021  1.00 19.11      A    O
ATOM    746  N   LEU A 103      -6.814  16.794  -4.959  1.00 19.97      A    N
ATOM    747  CA  LEU A 103      -6.225  15.634  -4.294  1.00 19.19      A    C
ATOM    748  CB  LEU A 103      -5.346  16.094  -3.131  1.00 18.87      A    C
ATOM    749  CG  LEU A 103      -4.169  16.986  -3.552  1.00 18.31      A    C
ATOM    750  CD1 LEU A 103      -3.298  17.397  -2.354  1.00 17.54      A    C
ATOM    751  CD2 LEU A 103      -3.341  16.297  -4.607  1.00 19.64      A    C
ATOM    752  C   LEU A 103      -7.307  14.676  -3.809  1.00 19.31      A    C
ATOM    753  O   LEU A 103      -7.179  14.018  -2.750  1.00 18.44      A    O
ATOM    754  N   GLY A 104      -8.371  14.586  -4.604  1.00 18.93      A    N
ATOM    755  CA  GLY A 104      -9.537  13.780  -4.260  1.00 18.78      A    C
ATOM    756  C   GLY A 104      -9.259  12.298  -4.234  1.00 18.26      A    C
ATOM    757  O   GLY A 104     -10.078  11.506  -3.780  1.00 19.17      A    O
ATOM    758  N   GLY A 105      -8.094  11.886  -4.703  1.00 17.54      A    N
ATOM    759  CA  GLY A 105      -7.698  10.500  -4.520  1.00 17.23      A    C
ATOM    760  C   GLY A 105      -7.395  10.091  -3.075  1.00 16.85      A    C
ATOM    761  O   GLY A 105      -7.319   8.895  -2.731  1.00 15.88      A    O
ATOM    762  N   LEU A 106      -7.263  11.067  -2.194  1.00 16.62      A    N
ATOM    763  CA  LEU A 106      -7.137  10.729  -0.777  1.00 16.79      A    C
ATOM    764  CB  LEU A 106      -6.892  11.975   0.048  1.00 16.05      A    C
ATOM    765  CG  LEU A 106      -5.519  12.560  -0.204  1.00 14.68      A    C
ATOM    766  CD1 LEU A 106      -5.479  13.986   0.274  1.00 16.20      A    C
ATOM    767  CD2 LEU A 106      -4.425  11.707   0.507  1.00 13.15      A    C
ATOM    768  C   LEU A 106      -8.423  10.056  -0.304  1.00 17.90      A    C
ATOM    769  O   LEU A 106      -9.513  10.553  -0.587  1.00 18.63      A    O
ATOM    770  N   PRO A 107      -8.318   8.932   0.387  1.00 18.42      A    N
ATOM    771  CA  PRO A 107      -9.506   8.280   0.977  1.00 19.35      A    C
ATOM    772  CB  PRO A 107      -8.963   6.932   1.430  1.00 19.15      A    C
ATOM    773  CG  PRO A 107      -7.537   7.286   1.774  1.00 19.19      A    C
ATOM    774  CD  PRO A 107      -7.089   8.162   0.640  1.00 18.63      A    C
ATOM    775  C   PRO A 107     -10.070   9.036   2.178  1.00 18.88      A    C
ATOM    776  O   PRO A 107      -9.340   9.724   2.886  1.00 19.33      A    O
ATOM    777  N   ALA A 108     -11.367   8.910   2.408  1.00 19.46      A    N
ATOM    778  CA  ALA A 108     -12.022   9.562   3.530  1.00 19.50      A    C
ATOM    779  CB  ALA A 108     -13.514   9.168   3.585  1.00 20.76      A    C
ATOM    780  C   ALA A 108     -11.359   9.229   4.875  1.00 18.72      A    C
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ATOM    781  O   ALA A 108     -11.229  10.093   5.727  1.00 19.17      A    O
ATOM    782  N   ASN A 109     -11.007   7.964   5.069  1.00 18.94      A    N
ATOM    783  CA  ASN A 109     -10.193   7.535   6.209  1.00 19.10      A    C
ATOM    784  CB  ASN A 109     -10.691   6.206   6.773  1.00 19.41      A    C
ATOM    785  CG  ASN A 109      -9.990   5.834   8.073  1.00 22.66      A    C
ATOM    786  OD1 ASN A 109      -8.872   6.295   8.349  1.00 19.31      A    O
ATOM    787  ND2 ASN A 109     -10.665   5.018   8.908  1.00 25.73      A    N
ATOM    788  C   ASN A 109      -8.731   7.392   5.804  1.00 17.97      A    C
ATOM    789  O   ASN A 109      -8.353   6.446   5.088  1.00 17.31      A    O
ATOM    790  N   LEU A 110      -7.895   8.325   6.245  1.00 16.66      A    N
ATOM    791  CA  LEU A 110      -6.489   8.277   5.862  1.00 15.50      A    C
ATOM    792  CB  LEU A 110      -5.738   9.502   6.406  1.00 15.65      A    C
ATOM    793  CG  LEU A 110      -6.096  10.831   5.749  1.00 13.74      A    C
ATOM    794  CD1 LEU A 110      -5.294  11.932   6.373  1.00 16.06      A    C
ATOM    795  CD2 LEU A 110      -5.873  10.768   4.256  1.00 13.53      A    C
ATOM    796  C   LEU A 110      -5.784   7.006   6.285  1.00 15.96      A    C
ATOM    797  O   LEU A 110      -4.750   6.660   5.719  1.00 16.04      A    O
ATOM    798  N   GLN A 111      -6.297   6.283   7.276  1.00 16.18      A    N
ATOM    799  CA  GLN A 111      -5.635   5.034   7.655  1.00 16.61      A    C
ATOM    800  CB  GLN A 111      -6.317   4.377   8.871  1.00 17.82      A    C
ATOM    801  CG  GLN A 111      -6.337   5.320  10.077  1.00 17.25      A    C
ATOM    802  CD  GLN A 111      -6.584   4.625  11.399  1.00 20.40      A    C
ATOM    803  OE1 GLN A 111      -5.934   3.635  11.699  1.00 21.99      A    O
ATOM    804  NE2 GLN A 111      -7.513   5.163  12.202  1.00 19.23      A    N
ATOM    805  C   GLN A 111      -5.560   4.086   6.461  1.00 17.45      A    C
ATOM    806  O   GLN A 111      -4.601   3.323   6.312  1.00 17.74      A    O
ATOM    807  N   THR A 112      -6.522   4.195   5.548  1.00 16.47      A    N
ATOM    808  CA  THR A 112      -6.483   3.418   4.309  1.00 16.12      A    C
ATOM    809  CB  THR A 112      -7.756   3.733   3.510  1.00 16.21      A    C
ATOM    810  OG1 THR A 112      -8.900   3.480   4.333  1.00 17.07      A    O
ATOM    811  CG2 THR A 112      -7.909   2.838   2.305  1.00 16.70      A    C
ATOM    812  C   THR A 112      -5.252   3.711   3.442  1.00 15.86      A    C
ATOM    813  O   THR A 112      -4.623   2.789   2.869  1.00 15.50      A    O
ATOM    814  N   LEU A 113      -4.933   4.995   3.303  1.00 14.75      A    N
ATOM    815  CA  LEU A 113      -3.742   5.413   2.558  1.00 14.05      A    C
ATOM    816  CB  LEU A 113      -3.677   6.941   2.557  1.00 14.27      A    C
ATOM    817  CG  LEU A 113      -2.549   7.597   1.807  1.00 14.53      A    C
ATOM    818  CD1 LEU A 113      -2.840   7.473   0.297  1.00 16.65      A    C
ATOM    819  CD2 LEU A 113      -2.412   9.039   2.212  1.00 13.95      A    C
ATOM    820  C   LEU A 113      -2.478   4.836   3.212  1.00 13.77      A    C
ATOM    821  O   LEU A 113      -1.625   4.238   2.550  1.00 13.55      A    O
ATOM    822  N   PHE A 114      -2.361   5.016   4.523  1.00 12.95      A    N
ATOM    823  CA  PHE A 114      -1.182   4.528   5.223  1.00 13.04      A    C
ATOM    824  CB  PHE A 114      -1.154   5.049   6.645  1.00 12.56      A    C
ATOM    825  CG  PHE A 114      -1.331   6.551   6.743  1.00 11.79      A    C
ATOM    826  CD1 PHE A 114      -0.639   7.402   5.902  1.00 12.07      A    C
ATOM    827  CE1 PHE A 114      -0.785   8.781   5.986  1.00 12.47      A    C
ATOM    828  CZ  PHE A 114      -1.662   9.323   6.921  1.00 13.57      A    C
ATOM    829  CE2 PHE A 114      -2.365   8.470   7.754  1.00 11.94      A    C
ATOM    830  CD2 PHE A 114      -2.186   7.100   7.663  1.00  9.85      A    C
ATOM    831  C   PHE A 114      -1.060   3.003   5.171  1.00 13.86      A    C
ATOM    832  O   PHE A 114       0.063   2.461   5.004  1.00 12.73      A    O
ATOM    833  N   SER A 115      -2.196   2.306   5.277  1.00 14.04      A    N
ATOM    834  CA  SER A 115      -2.148   0.848   5.292  1.00 14.17      A    C
ATOM    835  CB BSER A 115      -3.527   0.252   5.640  0.50 13.81      A    C
ATOM    836  CB ASER A 115      -3.457   0.215   5.769  0.50 14.55      A    C
ATOM    837  OG BSER A 115      -3.970   0.566   6.958  0.50 10.51      A    O
ATOM    838  OG ASER A 115      -4.544   0.608   4.978  0.50 18.03      A    O
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ATOM	839	C	SER	A	115	-1.677	0.296	3.943	1.00	14.11	A	C
ATOM	840	O	SER	A	115	-0.932	-0.663	3.909	1.00	13.43	A	O
ATOM	841	N	GLN	A	116	-2.108	0.890	2.832	1.00	14.73	A	N
ATOM	842	CA	GLN	A	116	-1.656	0.442	1.513	1.00	14.53	A	C
ATOM	843	CB	GLN	A	116	-2.394	1.234	0.417	1.00	15.81	A	C
ATOM	844	CG	GLN	A	116	-1.947	0.951	-1.038	1.00	15.88	A	C
ATOM	845	CD	GLN	A	116	-2.601	1.886	-2.007	1.00	16.75	A	C
ATOM	846	OE1	GLN	A	116	-2.629	3.086	-1.747	1.00	14.56	A	O
ATOM	847	NE2	GLN	A	116	-3.200	1.346	-3.106	1.00	14.07	A	N
ATOM	848	C	GLN	A	116	-0.131	0.571	1.375	1.00	14.16	A	C
ATOM	849	O	GLN	A	116	0.554	-0.336	0.861	1.00	14.37	A	O
ATOM	850	N	ALA	A	117	0.407	1.679	1.862	1.00	13.34	A	N
ATOM	851	CA	ALA	A	117	1.838	1.930	1.795	1.00	13.79	A	C
ATOM	852	CB	ALA	A	117	2.152	3.408	2.151	1.00	13.52	A	C
ATOM	853	C	ALA	A	117	2.608	0.972	2.714	1.00	13.17	A	C
ATOM	854	O	ALA	A	117	3.666	0.472	2.344	1.00	13.07	A	O
ATOM	855	N	TYR	A	118	2.071	0.740	3.908	1.00	13.32	A	N
ATOM	856	CA	TYR	A	118	2.679	-0.161	4.877	1.00	13.82	A	C
ATOM	857	CB	TYR	A	118	1.878	-0.177	6.190	1.00	14.02	A	C
ATOM	858	CG	TYR	A	118	2.636	-0.861	7.324	1.00	17.04	A	C
ATOM	859	CD1	TYR	A	118	2.472	-2.216	7.589	1.00	20.14	A	C
ATOM	860	CE1	TYR	A	118	3.186	-2.839	8.640	1.00	24.14	A	C
ATOM	861	CZ	TYR	A	118	4.041	-2.071	9.409	1.00	23.61	A	C
ATOM	862	OH	TYR	A	118	4.762	-2.631	10.442	1.00	28.49	A	O
ATOM	863	CE2	TYR	A	118	4.194	-0.725	9.155	1.00	20.69	A	C
ATOM	864	CD2	TYR	A	118	3.501	-0.135	8.136	1.00	18.61	A	C
ATOM	865	C	TYR	A	118	2.782	-1.576	4.294	1.00	14.18	A	C
ATOM	866	O	TYR	A	118	3.838	-2.228	4.363	1.00	14.05	A	O
ATOM	867	N	SER	A	119	1.705	-2.024	3.669	1.00	14.24	A	N
ATOM	868	CA	SER	A	119	1.684	-3.358	3.064	1.00	15.13	A	C
ATOM	869	CB	SER	A	119	0.288	-3.660	2.544	1.00	14.77	A	C
ATOM	870	OG	SER	A	119	-0.609	-3.744	3.638	1.00	13.56	A	O
ATOM	871	C	SER	A	119	2.752	-3.531	1.977	1.00	15.67	A	C
ATOM	872	O	SER	A	119	3.313	-4.602	1.818	1.00	15.80	A	O
ATOM	873	N	ALA	A	120	3.052	-2.461	1.254	1.00	16.24	A	N
ATOM	874	CA	ALA	A	120	4.085	-2.488	0.204	1.00	15.93	A	C
ATOM	875	CB	ALA	A	120	3.847	-1.352	-0.759	1.00	16.16	A	C
ATOM	876	C	ALA	A	120	5.504	-2.405	0.767	1.00	16.13	A	C
ATOM	877	O	ALA	A	120	6.474	-2.473	0.030	1.00	16.93	A	O
ATOM	878	N	GLY	A	121	5.626	-2.249	2.083	1.00	16.23	A	N
ATOM	879	CA	GLY	A	121	6.917	-2.249	2.747	1.00	15.35	A	C
ATOM	880	C	GLY	A	121	7.400	-0.883	3.247	1.00	15.15	A	C
ATOM	881	O	GLY	A	121	8.466	-0.811	3.893	1.00	15.57	A	O
ATOM	882	N	ALA	A	122	6.665	0.195	2.977	1.00	14.40	A	N
ATOM	883	CA	ALA	A	122	7.110	1.522	3.443	1.00	14.85	A	C
ATOM	884	CB	ALA	A	122	6.273	2.632	2.831	1.00	14.84	A	C
ATOM	885	C	ALA	A	122	7.057	1.635	4.964	1.00	14.35	A	C
ATOM	886	O	ALA	A	122	6.078	1.230	5.574	1.00	15.21	A	O
ATOM	887	N	ARG	A	123	8.077	2.223	5.570	1.00	13.62	A	N
ATOM	888	CA	ARG	A	123	8.013	2.499	7.008	1.00	12.85	A	C
ATOM	889	CB	ARG	A	123	9.065	1.689	7.761	1.00	12.85	A	C
ATOM	890	CG	ARG	A	123	8.870	0.162	7.597	1.00	13.74	A	C
ATOM	891	CD	ARG	A	123	7.584	-0.334	8.290	1.00	14.35	A	C
ATOM	892	NE	ARG	A	123	7.396	-1.786	8.187	1.00	14.77	A	N
ATOM	893	CZ	ARG	A	123	6.676	-2.389	7.253	1.00	16.63	A	C
ATOM	894	NH1	ARG	A	123	6.039	-1.678	6.337	1.00	15.68	A	N
ATOM	895	NH2	ARG	A	123	6.579	-3.719	7.240	1.00	17.36	A	N
ATOM	896	C	ARG	A	123	8.132	3.987	7.298	1.00	12.72	A	C

ATOM	897	O	ARG	A	123	8.116	4.418	8.448	1.00	12.15	A	O
ATOM	898	N	ILE	A	124	8.225	4.773	6.234	1.00	12.67	A	N
ATOM	899	CA	ILE	A	124	8.177	6.218	6.346	1.00	12.97	A	C
ATOM	900	CB	ILE	A	124	9.554	6.814	6.025	1.00	12.64	A	C
ATOM	901	CG1	ILE	A	124	10.619	6.262	6.985	1.00	13.71	A	C
ATOM	902	CD1	ILE	A	124	12.068	6.395	6.480	1.00	14.82	A	C
ATOM	903	CG2	ILE	A	124	9.478	8.348	6.061	1.00	13.97	A	C
ATOM	904	C	ILE	A	124	7.160	6.695	5.324	1.00	12.91	A	C
ATOM	905	O	ILE	A	124	7.132	6.195	4.210	1.00	13.07	A	O
ATOM	906	N	HIS	A	125	6.365	7.696	5.671	1.00	12.94	A	N
ATOM	907	CA	HIS	A	125	5.252	8.100	4.823	1.00	12.77	A	C
ATOM	908	CB	HIS	A	125	3.894	7.549	5.353	1.00	13.00	A	C
ATOM	909	CG	HIS	A	125	2.806	7.650	4.334	1.00	15.91	A	C
ATOM	910	ND1	HIS	A	125	2.428	8.850	3.783	1.00	13.47	A	N
ATOM	911	CE1	HIS	A	125	1.547	8.632	2.821	1.00	16.40	A	C
ATOM	912	NE2	HIS	A	125	1.312	7.333	2.756	1.00	16.49	A	N
ATOM	913	CD2	HIS	A	125	2.072	6.699	3.705	1.00	18.35	A	C
ATOM	914	C	HIS	A	125	5.223	9.620	4.828	1.00	12.62	A	C
ATOM	915	O	HIS	A	125	5.053	10.202	5.893	1.00	12.04	A	O
ATOM	916	N	THR	A	126	5.401	10.268	3.674	1.00	12.71	A	N
ATOM	917	CA	THR	A	126	5.527	11.738	3.641	1.00	12.63	A	C
ATOM	918	CB	THR	A	126	6.984	12.142	3.302	1.00	12.63	A	C
ATOM	919	OG1	THR	A	126	7.121	13.560	3.334	1.00	12.18	A	O
ATOM	920	CG2	THR	A	126	7.395	11.747	1.864	1.00	12.36	A	C
ATOM	921	C	THR	A	126	4.498	12.426	2.735	1.00	12.60	A	C
ATOM	922	O	THR	A	126	4.166	11.931	1.652	1.00	12.62	A	O
ATOM	923	N	ASN	A	127	4.010	13.572	3.200	1.00	12.52	A	N
ATOM	924	CA	ASN	A	127	2.778	14.189	2.696	1.00	12.84	A	C
ATOM	925	CB	ASN	A	127	1.599	13.811	3.605	1.00	13.04	A	C
ATOM	926	CG	ASN	A	127	1.433	12.325	3.720	1.00	13.25	A	C
ATOM	927	OD1	ASN	A	127	1.916	11.686	4.690	1.00	13.15	A	O
ATOM	928	ND2	ASN	A	127	0.814	11.740	2.712	1.00	9.82	A	N
ATOM	929	C	ASN	A	127	2.894	15.706	2.637	1.00	12.70	A	C
ATOM	930	O	ASN	A	127	2.798	16.390	3.661	1.00	13.27	A	O
ATOM	931	N	SER	A	128	3.103	16.211	1.435	1.00	12.76	A	N
ATOM	932	CA	SER	A	128	3.277	17.640	1.162	1.00	13.02	A	C
ATOM	933	CB	SER	A	128	4.308	17.831	0.043	1.00	12.57	A	C
ATOM	934	OG	SER	A	128	5.608	17.510	0.485	1.00	12.52	A	O
ATOM	935	C	SER	A	128	1.927	18.238	0.748	1.00	13.42	A	C
ATOM	936	O	SER	A	128	1.763	18.767	-0.372	1.00	13.82	A	O
ATOM	937	N	TRP	A	129	0.968	18.129	1.663	1.00	13.86	A	N
ATOM	938	CA	TRP	A	129	-0.392	18.616	1.465	1.00	13.67	A	C
ATOM	939	CB	TRP	A	129	-1.215	17.648	0.602	1.00	13.88	A	C
ATOM	940	CG	TRP	A	129	-1.130	16.180	0.964	1.00	13.08	A	C
ATOM	941	CD1	TRP	A	129	-0.305	15.232	0.391	1.00	14.80	A	C
ATOM	942	NE1	TRP	A	129	-0.531	13.997	0.956	1.00	12.40	A	N
ATOM	943	CE2	TRP	A	129	-1.518	14.122	1.900	1.00	13.40	A	C
ATOM	944	CD2	TRP	A	129	-1.924	15.480	1.921	1.00	12.64	A	C
ATOM	945	CE3	TRP	A	129	-2.948	15.857	2.806	1.00	14.15	A	C
ATOM	946	CZ3	TRP	A	129	-3.504	14.910	3.614	1.00	13.25	A	C
ATOM	947	CH2	TRP	A	129	-3.082	13.566	3.559	1.00	13.78	A	C
ATOM	948	CZ2	TRP	A	129	-2.101	13.158	2.711	1.00	12.56	A	C
ATOM	949	C	TRP	A	129	-1.089	18.859	2.782	1.00	14.44	A	C
ATOM	950	O	TRP	A	129	-0.612	18.460	3.876	1.00	14.19	A	O
ATOM	951	N	GLY	A	130	-2.224	19.538	2.694	1.00	14.75	A	N
ATOM	952	CA	GLY	A	130	-3.004	19.834	3.866	1.00	15.45	A	C
ATOM	953	C	GLY	A	130	-4.173	20.744	3.563	1.00	16.66	A	C
ATOM	954	O	GLY	A	130	-4.203	21.394	2.518	1.00	16.04	A	O

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ATOM    955  N   ALA A 131      -5.139  20.754   4.478  1.00 16.87      A    N
ATOM    956  CA  ALA A 131      -6.222  21.733   4.484  1.00 18.19      A    C
ATOM    957  CB  ALA A 131      -7.515  21.097   4.983  1.00 17.33      A    C
ATOM    958  C   ALA A 131      -5.843  22.852   5.423  1.00 19.54      A    C
ATOM    959  O   ALA A 131      -5.562  22.590   6.592  1.00 20.18      A    O
ATOM    960  N   PRO A 132      -5.869  24.090   4.942  1.00 20.97      A    N
ATOM    961  CA  PRO A 132      -5.513  25.253   5.763  1.00 21.46      A    C
ATOM    962  CB  PRO A 132      -5.260  26.346   4.724  1.00 21.95      A    C
ATOM    963  CG  PRO A 132      -6.060  25.967   3.546  1.00 22.18      A    C
ATOM    964  CD  PRO A 132      -6.220  24.462   3.564  1.00 21.43      A    C
ATOM    965  C   PRO A 132      -6.595  25.676   6.753  1.00 22.74      A    C
ATOM    966  O   PRO A 132      -7.272  26.703   6.555  1.00 24.13      A    O
ATOM    967  N   VAL A 133      -6.708  24.912   7.833  1.00 22.71      A    N
ATOM    968  CA  VAL A 133      -7.723  25.086   8.850  1.00 23.39      A    C
ATOM    969  CB  VAL A 133      -8.349  23.712   9.223  1.00 23.48      A    C
ATOM    970  CG1 VAL A 133      -9.115  23.133   8.045  1.00 25.68      A    C
ATOM    971  CG2 VAL A 133      -7.269  22.750   9.687  1.00 24.53      A    C
ATOM    972  C   VAL A 133      -7.223  25.742  10.150  1.00 23.23      A    C
ATOM    973  O   VAL A 133      -7.855  25.599  11.185  1.00 22.57      A    O
ATOM    974  N   ASN A 134      -6.094  26.437  10.098  1.00 23.10      A    N
ATOM    975  CA  ASN A 134      -5.660  27.279  11.201  1.00 23.36      A    C
ATOM    976  CB  ASN A 134      -6.583  28.512  11.310  1.00 24.40      A    C
ATOM    977  CG  ASN A 134      -6.491  29.413  10.082  1.00 26.68      A    C
ATOM    978  OD1 ASN A 134      -7.489  30.000   9.650  1.00 34.40      A    O
ATOM    979  ND2 ASN A 134      -5.315  29.478   9.482  1.00 28.87      A    N
ATOM    980  C   ASN A 134      -5.588  26.561  12.535  1.00 22.43      A    C
ATOM    981  O   ASN A 134      -6.210  26.971  13.510  1.00 21.30      A    O
ATOM    982  N   GLY A 135      -4.844  25.458  12.574  1.00 21.06      A    N
ATOM    983  CA  GLY A 135      -4.548  24.840  13.846  1.00 20.36      A    C
ATOM    984  C   GLY A 135      -5.541  23.818  14.308  1.00 19.66      A    C
ATOM    985  O   GLY A 135      -5.320  23.200  15.327  1.00 18.95      A    O
ATOM    986  N   ALA A 136      -6.613  23.595  13.557  1.00 19.08      A    N
ATOM    987  CA  ALA A 136      -7.609  22.643  14.006  1.00 19.00      A    C
ATOM    988  CB  ALA A 136      -8.925  22.778  13.199  1.00 19.34      A    C
ATOM    989  C   ALA A 136      -7.098  21.206  13.893  1.00 19.31      A    C
ATOM    990  O   ALA A 136      -6.354  20.851  12.952  1.00 18.44      A    O
ATOM    991  N   TYR A 137      -7.568  20.407  14.841  1.00 18.56      A    N
ATOM    992  CA  TYR A 137      -7.341  18.979  14.907  1.00 18.99      A    C
ATOM    993  CB  TYR A 137      -7.112  18.588  16.367  1.00 18.67      A    C
ATOM    994  CG  TYR A 137      -6.637  17.175  16.588  1.00 19.68      A    C
ATOM    995  CD1 TYR A 137      -7.537  16.173  16.885  1.00 19.55      A    C
ATOM    996  CE1 TYR A 137      -7.112  14.855  17.099  1.00 21.07      A    C
ATOM    997  CZ  TYR A 137      -5.765  14.548  17.045  1.00 20.92      A    C
ATOM    998  OH  TYR A 137      -5.371  13.250  17.265  1.00 20.20      A    O
ATOM    999  CE2 TYR A 137      -4.837  15.538  16.754  1.00 20.35      A    C
ATOM   1000  CD2 TYR A 137      -5.278  16.848  16.522  1.00 19.75      A    C
ATOM   1001  C   TYR A 137      -8.600  18.314  14.337  1.00 18.91      A    C
ATOM   1002  O   TYR A 137      -9.648  18.229  14.994  1.00 18.41      A    O
ATOM   1003  N   THR A 138      -8.481  17.872  13.091  1.00 18.62      A    N
ATOM   1004  CA  THR A 138      -9.608  17.401  12.329  1.00 17.86      A    C
ATOM   1005  CB  THR A 138      -9.480  17.836  10.897  1.00 18.02      A    C
ATOM   1006  OG1 THR A 138      -8.271  17.308  10.321  1.00 16.63      A    O
ATOM   1007  CG2 THR A 138      -9.308  19.330  10.788  1.00 17.63      A    C
ATOM   1008  C   THR A 138      -9.593  15.888  12.407  1.00 18.43      A    C
ATOM   1009  O   THR A 138      -8.662  15.296  12.954  1.00 17.82      A    O
ATOM   1010  N   THR A 139     -10.624  15.278  11.843  1.00 18.06      A    N
ATOM   1011  CA  THR A 139     -10.713  13.843  11.705  1.00 17.69      A    C
ATOM   1012  CB  THR A 139     -12.020  13.472  10.947  1.00 18.57      A    C
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ATOM   1013  OG1 THR A 139     -13.162  13.907  11.705  1.00 20.05      A    O
ATOM   1014  CG2 THR A 139     -12.173  11.933  10.828  1.00 19.16      A    C
ATOM   1015  C   THR A 139      -9.496  13.285  10.989  1.00 16.78      A    C
ATOM   1016  O   THR A 139      -9.037  12.183  11.307  1.00 17.05      A    O
ATOM   1017  N   ASP A 140      -8.976  14.002  10.002  1.00 15.81      A    N
ATOM   1018  CA  ASP A 140      -7.758  13.544   9.351  1.00 15.65      A    C
ATOM   1019  CB  ASP A 140      -7.391  14.429   8.177  1.00 15.45      A    C
ATOM   1020  CG  ASP A 140      -8.279  14.209   6.984  1.00 16.65      A    C
ATOM   1021  OD1 ASP A 140      -8.495  15.189   6.263  1.00 18.76      A    O
ATOM   1022  OD2 ASP A 140      -8.781  13.102   6.702  1.00 16.74      A    O
ATOM   1023  C   ASP A 140      -6.567  13.504  10.352  1.00 15.55      A    C
ATOM   1024  O   ASP A 140      -5.823  12.532  10.395  1.00 15.72      A    O
ATOM   1025  N   SER A 141      -6.395  14.555  11.133  1.00 15.34      A    N
ATOM   1026  CA  SER A 141      -5.375  14.548  12.187  1.00 15.53      A    C
ATOM   1027  CB  SER A 141      -5.428  15.823  13.006  1.00 14.57      A    C
ATOM   1028  OG  SER A 141      -5.275  16.936  12.173  1.00 16.14      A    O
ATOM   1029  C   SER A 141      -5.514  13.375  13.157  1.00 15.46      A    C
ATOM   1030  O   SER A 141      -4.511  12.754  13.558  1.00 15.37      A    O
ATOM   1031  N   ARG A 142      -6.754  13.100  13.546  1.00 15.27      A    N
ATOM   1032  CA  ARG A 142      -7.053  11.998  14.462  1.00 15.97      A    C
ATOM   1033  CB  ARG A 142      -8.539  12.004  14.843  1.00 16.78      A    C
ATOM   1034  CG  ARG A 142      -8.882  11.091  16.022  1.00 18.90      A    C
ATOM   1035  CD  ARG A 142     -10.365  11.103  16.436  1.00 22.40      A    C
ATOM   1036  NE  ARG A 142     -10.533  10.384  17.704  1.00 25.70      A    N
ATOM   1037  CZ  ARG A 142     -10.549   9.057  17.839  1.00 29.38      A    C
ATOM   1038  NH1 ARG A 142     -10.423   8.249  16.786  1.00 30.26      A    N
ATOM   1039  NH2 ARG A 142     -10.685   8.524  19.048  1.00 30.56      A    N
ATOM   1040  C   ARG A 142      -6.703  10.643  13.860  1.00 15.43      A    C
ATOM   1041  O   ARG A 142      -6.107   9.778  14.534  1.00 14.36      A    O
ATOM   1042  N   ASN A 143      -7.068  10.437  12.593  1.00 14.96      A    N
ATOM   1043  CA  ASN A 143      -6.699   9.187  11.926  1.00 14.70      A    C
ATOM   1044  CB  ASN A 143      -7.451   9.062  10.593  1.00 15.54      A    C
ATOM   1045  CG  ASN A 143      -8.952   8.709  10.803  1.00 16.85      A    C
ATOM   1046  OD1 ASN A 143      -9.842   9.204  10.096  1.00 20.66      A    O
ATOM   1047  ND2 ASN A 143      -9.206   7.828  11.746  1.00 15.73      A    N
ATOM   1048  C   ASN A 143      -5.183   8.986  11.754  1.00 15.26      A    C
ATOM   1049  O   ASN A 143      -4.691   7.854  11.879  1.00 15.15      A    O
ATOM   1050  N   VAL A 144      -4.438  10.060  11.450  1.00 14.90      A    N
ATOM   1051  CA  VAL A 144      -2.976   9.987  11.467  1.00 13.93      A    C
ATOM   1052  CB  VAL A 144      -2.319  11.347  11.177  1.00 14.08      A    C
ATOM   1053  CG1 VAL A 144      -0.803  11.272  11.422  1.00 12.32      A    C
ATOM   1054  CG2 VAL A 144      -2.625  11.818   9.748  1.00 13.08      A    C
ATOM   1055  C   VAL A 144      -2.478   9.507  12.843  1.00 14.23      A    C
ATOM   1056  O   VAL A 144      -1.608   8.653  12.938  1.00 13.96      A    O
ATOM   1057  N   ASP A 145      -3.021  10.077  13.916  1.00 14.48      A    N
ATOM   1058  CA  ASP A 145      -2.548   9.745  15.256  1.00 14.49      A    C
ATOM   1059  CB  ASP A 145      -3.123  10.711  16.249  1.00 14.81      A    C
ATOM   1060  CG  ASP A 145      -2.406  12.033  16.218  1.00 15.70      A    C
ATOM   1061  OD1 ASP A 145      -1.332  12.107  15.545  1.00 14.69      A    O
ATOM   1062  OD2 ASP A 145      -2.845  13.048  16.803  1.00 14.46      A    O
ATOM   1063  C   ASP A 145      -2.849   8.331  15.654  1.00 15.08      A    C
ATOM   1064  O   ASP A 145      -1.999   7.622  16.183  1.00 14.89      A    O
ATOM   1065  N   ASP A 146      -4.065   7.906  15.361  1.00 15.66      A    N
ATOM   1066  CA  ASP A 146      -4.470   6.545  15.608  1.00 15.98      A    C
ATOM   1067  CB  ASP A 146      -5.931   6.400  15.184  1.00 16.37      A    C
ATOM   1068  CG  ASP A 146      -6.565   5.107  15.705  1.00 17.81      A    C
ATOM   1069  OD1 ASP A 146      -6.337   4.735  16.879  1.00 18.17      A    O
ATOM   1070  OD2 ASP A 146      -7.277   4.401  14.981  1.00 21.66      A    O
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ATOM   1071  C   ASP A 146      -3.562   5.571  14.849  1.00 16.07      A    C
ATOM   1072  O   ASP A 146      -3.047   4.607  15.408  1.00 16.60      A    O
ATOM   1073  N   TYR A 147      -3.324   5.842  13.576  1.00 15.73      A    N
ATOM   1074  CA  TYR A 147      -2.463   4.988  12.772  1.00 15.49      A    C
ATOM   1075  CB  TYR A 147      -2.387   5.486  11.314  1.00 15.22      A    C
ATOM   1076  CG  TYR A 147      -1.759   4.421  10.459  1.00 16.31      A    C
ATOM   1077  CD1 TYR A 147      -0.400   4.394  10.249  1.00 17.35      A    C
ATOM   1078  CE1 TYR A 147       0.180   3.380   9.506  1.00 17.49      A    C
ATOM   1079  CZ  TYR A 147      -0.599   2.364   9.004  1.00 16.46      A    C
ATOM   1080  OH  TYR A 147      -0.022   1.354   8.281  1.00 20.80      A    O
ATOM   1081  CE2 TYR A 147      -1.944   2.346   9.227  1.00 16.19      A    C
ATOM   1082  CD2 TYR A 147      -2.523   3.364   9.947  1.00 16.98      A    C
ATOM   1083  C   TYR A 147      -1.025   4.833  13.309  1.00 15.68      A    C
ATOM   1084  O   TYR A 147      -0.491   3.719  13.385  1.00 14.79      A    O
ATOM   1085  N   VAL A 148      -0.399   5.953  13.652  1.00 16.33      A    N
ATOM   1086  CA  VAL A 148       0.975   5.950  14.144  1.00 16.18      A    C
ATOM   1087  CB  VAL A 148       1.534   7.390  14.262  1.00 16.37      A    C
ATOM   1088  CG1 VAL A 148       2.953   7.397  14.909  1.00 17.53      A    C
ATOM   1089  CG2 VAL A 148       1.600   8.044  12.899  1.00 16.39      A    C
ATOM   1090  C   VAL A 148       1.063   5.206  15.488  1.00 16.59      A    C
ATOM   1091  O   VAL A 148       2.022   4.481  15.765  1.00 16.63      A    O
ATOM   1092  N   ARG A 149       0.061   5.356  16.331  1.00 16.70      A    N
ATOM   1093  CA  ARG A 149       0.109   4.628  17.589  1.00 18.28      A    C
ATOM   1094  CB  ARG A 149      -0.920   5.133  18.600  1.00 18.33      A    C
ATOM   1095  CG  ARG A 149      -0.585   4.657  20.002  1.00 19.51      A    C
ATOM   1096  CD  ARG A 149      -1.566   5.035  21.071  1.00 20.84      A    C
ATOM   1097  NE  ARG A 149      -0.987   4.731  22.383  1.00 22.92      A    N
ATOM   1098  CZ  ARG A 149      -1.661   4.491  23.504  1.00 24.06      A    C
ATOM   1099  NH1 ARG A 149      -2.985   4.521  23.538  1.00 25.69      A    N
ATOM   1100  NH2 ARG A 149      -0.987   4.221  24.616  1.00 23.61      A    N
ATOM   1101  C   ARG A 149      -0.035   3.126  17.382  1.00 18.63      A    C
ATOM   1102  O   ARG A 149       0.517   2.346  18.156  1.00 18.97      A    O
ATOM   1103  N   LYS A 150      -0.739   2.720  16.326  1.00 18.98      A    N
ATOM   1104  CA  LYS A 150      -0.991   1.294  16.087  1.00 19.24      A    C
ATOM   1105  CB  LYS A 150      -2.373   1.092  15.438  1.00 19.89      A    C
ATOM   1106  CG  LYS A 150      -3.576   1.358  16.389  1.00 21.34      A    C
ATOM   1107  CD  LYS A 150      -4.902   0.972  15.736  1.00 24.20      A    C
ATOM   1108  CE  LYS A 150      -6.136   1.437  16.531  1.00 27.20      A    C
ATOM   1109  NZ  LYS A 150      -7.373   1.614  15.668  1.00 30.36      A    N
ATOM   1110  C   LYS A 150       0.123   0.622  15.250  1.00 18.99      A    C
ATOM   1111  O   LYS A 150       0.296  -0.577  15.305  1.00 17.16      A    O
ATOM   1112  N   ASN A 151       0.916   1.407  14.526  1.00 19.09      A    N
ATOM   1113  CA  ASN A 151       1.834   0.850  13.538  1.00 19.75      A    C
ATOM   1114  CB  ASN A 151       1.225   0.950  12.130  1.00 20.10      A    C
ATOM   1115  CG  ASN A 151      -0.141   0.299  12.025  1.00 19.86      A    C
ATOM   1116  OD1 ASN A 151      -0.239  -0.905  11.855  1.00 19.33      A    O
ATOM   1117  ND2 ASN A 151      -1.198   1.090  12.167  1.00 19.31      A    N
ATOM   1118  C   ASN A 151       3.150   1.599  13.557  1.00 20.21      A    C
ATOM   1119  O   ASN A 151       3.193   2.807  13.793  1.00 22.14      A    O
ATOM   1120  N   ASP A 152       4.239   0.911  13.299  1.00 20.04      A    N
ATOM   1121  CA  ASP A 152       5.508   1.595  13.319  1.00 20.51      A    C
ATOM   1122  CB BASP A 152       6.571   0.640  13.830  0.35 20.16      A    C
ATOM   1123  CB AASP A 152       6.645   0.666  13.762  0.65 21.56      A    C
ATOM   1124  CG BASP A 152       6.199   0.067  15.205  0.35 19.09      A    C
ATOM   1125  CG AASP A 152       7.225  -0.117  12.631  0.65 23.76      A    C
ATOM   1126  OD1BASP A 152       5.318   0.654  15.901  0.35 15.06      A    O
ATOM   1127  OD1AASP A 152       6.404  -0.719  11.924  0.65 27.77      A    O
ATOM   1128  OD2BASP A 152       6.703  -0.977  15.653  0.35 16.81      A    O
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ATOM   1129  OD2AASP A 152       8.471  -0.170  12.353  0.65 27.40      A    O
ATOM   1130  C    ASP A 152       5.822   2.270  11.959  1.00 19.32      A    C
ATOM   1131  O    ASP A 152       6.748   1.916  11.253  1.00 20.60      A    O
ATOM   1132  N    MET A 153       4.988   3.250  11.628  1.00 16.58      A    N
ATOM   1133  CA   MET A 153       5.154   4.050  10.437  1.00 16.03      A    C
ATOM   1134  CB   MET A 153       3.876   4.007   9.619  1.00 16.23      A    C
ATOM   1135  CG   MET A 153       3.885   4.921   8.432  1.00 18.33      A    C
ATOM   1136  SD   MET A 153       4.694   4.182   7.030  1.00 21.72      A    S
ATOM   1137  CE   MET A 153       3.290   3.549   6.297  1.00 21.74      A    C
ATOM   1138  C    MET A 153       5.443   5.482  10.871  1.00 14.80      A    C
ATOM   1139  O    MET A 153       4.684   6.058  11.646  1.00 13.50      A    O
ATOM   1140  N    THR A 154       6.525   6.059  10.368  1.00 13.34      A    N
ATOM   1141  CA   THR A 154       6.813   7.482  10.638  1.00 13.08      A    C
ATOM   1142  CB   THR A 154       8.324   7.699  10.652  1.00 13.02      A    C
ATOM   1143  OG1  THR A 154       8.886   6.949  11.724  1.00 11.51      A    O
ATOM   1144  CG2  THR A 154       8.693   9.145  10.963  1.00 14.36      A    C
ATOM   1145  C    THR A 154       6.153   8.310   9.573  1.00 12.50      A    C
ATOM   1146  O    THR A 154       6.396   8.108   8.371  1.00 12.64      A    O
ATOM   1147  N    ILE A 155       5.290   9.227   9.987  1.00 12.34      A    N
ATOM   1148  CA   ILE A 155       4.492  10.002   9.037  1.00 13.00      A    C
ATOM   1149  CB   ILE A 155       2.983   9.799   9.346  1.00 13.05      A    C
ATOM   1150  CG1  ILE A 155       2.637   8.307   9.279  1.00 13.73      A    C
ATOM   1151  CD1  ILE A 155       1.121   8.017   9.274  1.00 12.93      A    C
ATOM   1152  CG2  ILE A 155       2.121  10.578   8.371  1.00 13.58      A    C
ATOM   1153  C    ILE A 155       4.861  11.480   9.137  1.00 13.01      A    C
ATOM   1154  O    ILE A 155       4.894  12.038  10.233  1.00 12.79      A    O
ATOM   1155  N    LEU A 156       5.125  12.117   8.001  1.00 12.16      A    N
ATOM   1156  CA   LEU A 156       5.509  13.528   7.982  1.00 12.88      A    C
ATOM   1157  CB   LEU A 156       6.903  13.692   7.354  1.00 12.18      A    C
ATOM   1158  CG   LEU A 156       8.089  12.960   8.007  1.00 13.25      A    C
ATOM   1159  CD1  LEU A 156       8.365  11.607   7.326  1.00 11.24      A    C
ATOM   1160  CD2  LEU A 156       9.339  13.796   7.910  1.00 13.01      A    C
ATOM   1161  C    LEU A 156       4.485  14.328   7.192  1.00 13.49      A    C
ATOM   1162  O    LEU A 156       3.982  13.850   6.160  1.00 14.76      A    O
ATOM   1163  N    PHE A 157       4.197  15.540   7.659  1.00 12.79      A    N
ATOM   1164  CA   PHE A 157       3.282  16.451   7.003  1.00 13.07      A    C
ATOM   1165  CB   PHE A 157       1.938  16.564   7.772  1.00 13.62      A    C
ATOM   1166  CG   PHE A 157       0.957  15.504   7.401  1.00 13.90      A    C
ATOM   1167  CD1  PHE A 157       0.191  15.636   6.272  1.00 11.22      A    C
ATOM   1168  CE1  PHE A 157      -0.678  14.632   5.896  1.00 14.22      A    C
ATOM   1169  CZ   PHE A 157      -0.743  13.441   6.630  1.00 14.61      A    C
ATOM   1170  CE2  PHE A 157       0.013  13.296   7.743  1.00 15.64      A    C
ATOM   1171  CD2  PHE A 157       0.891  14.312   8.122  1.00 14.56      A    C
ATOM   1172  C    PHE A 157       3.899  17.852   6.928  1.00 13.18      A    C
ATOM   1173  O    PHE A 157       4.527  18.318   7.867  1.00 12.04      A    O
ATOM   1174  N    ALA A 158       3.700  18.500   5.793  1.00 13.46      A    N
ATOM   1175  CA   ALA A 158       3.958  19.921   5.623  1.00 13.31      A    C
ATOM   1176  CB   ALA A 158       3.509  20.334   4.235  1.00 14.02      A    C
ATOM   1177  C    ALA A 158       3.181  20.703   6.672  1.00 13.75      A    C
ATOM   1178  O    ALA A 158       2.031  20.380   6.965  1.00 13.75      A    O
ATOM   1179  N    ALA A 159       3.787  21.752   7.215  1.00 13.45      A    N
ATOM   1180  CA   ALA A 159       3.122  22.582   8.210  1.00 13.81      A    C
ATOM   1181  CB   ALA A 159       4.151  23.495   8.944  1.00 13.64      A    C
ATOM   1182  C    ALA A 159       2.043  23.473   7.628  1.00 14.14      A    C
ATOM   1183  O    ALA A 159       1.175  23.924   8.364  1.00 14.00      A    O
ATOM   1184  N    GLY A 160       2.131  23.753   6.330  1.00 15.19      A    N
ATOM   1185  CA   GLY A 160       1.230  24.680   5.652  1.00 15.34      A    C
ATOM   1186  C    GLY A 160       1.957  25.941   5.236  1.00 14.93      A    C
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ATOM   1187  O   GLY A 160       3.041  26.238   5.736  1.00 14.62      A    O
ATOM   1188  N   ASN A 161       1.371  26.686   4.307  1.00 15.04      A    N
ATOM   1189  CA  ASN A 161       1.983  27.902   3.789  1.00 15.84      A    C
ATOM   1190  CB  ASN A 161       2.072  27.872   2.261  1.00 15.91      A    C
ATOM   1191  CG  ASN A 161       3.048  26.851   1.712  1.00 17.40      A    C
ATOM   1192  OD1 ASN A 161       3.001  26.550   0.490  1.00 21.70      A    O
ATOM   1193  ND2 ASN A 161       3.888  26.267   2.569  1.00 11.15      A    N
ATOM   1194  C   ASN A 161       1.131  29.114   4.123  1.00 16.84      A    C
ATOM   1195  O   ASN A 161       0.956  29.965   3.286  1.00 17.07      A    O
ATOM   1196  N   GLU A 162       0.575  29.179   5.324  1.00 18.36      A    N
ATOM   1197  CA  GLU A 162      -0.392  30.213   5.668  1.00 18.85      A    C
ATOM   1198  CB  GLU A 162      -1.672  29.537   6.211  1.00 19.64      A    C
ATOM   1199  CG  GLU A 162      -2.431  28.723   5.150  1.00 22.12      A    C
ATOM   1200  CD  GLU A 162      -1.756  27.381   4.788  1.00 26.12      A    C
ATOM   1201  OE1 GLU A 162      -1.585  26.545   5.702  1.00 28.48      A    O
ATOM   1202  OE2 GLU A 162      -1.405  27.149   3.590  1.00 26.75      A    O
ATOM   1203  C   GLU A 162       0.147  31.262   6.657  1.00 19.39      A    C
ATOM   1204  O   GLU A 162      -0.633  32.031   7.225  1.00 18.80      A    O
ATOM   1205  N   GLY A 163       1.472  31.338   6.820  1.00 19.39      A    N
ATOM   1206  CA  GLY A 163       2.082  32.322   7.705  1.00 20.03      A    C
ATOM   1207  C   GLY A 163       2.224  33.699   7.048  1.00 21.41      A    C
ATOM   1208  O   GLY A 163       1.822  33.866   5.877  1.00 20.72      A    O
ATOM   1209  N   PRO A 164       2.835  34.671   7.737  1.00 21.93      A    N
ATOM   1210  CA  PRO A 164       3.496  34.491   9.053  1.00 22.22      A    C
ATOM   1211  CB  PRO A 164       4.575  35.577   9.050  1.00 22.99      A    C
ATOM   1212  CG  PRO A 164       3.945  36.720   8.171  1.00 23.13      A    C
ATOM   1213  CD  PRO A 164       2.976  36.047   7.209  1.00 22.03      A    C
ATOM   1214  C   PRO A 164       2.681  34.621  10.329  1.00 22.18      A    C
ATOM   1215  O   PRO A 164       3.289  34.603  11.414  1.00 21.36      A    O
ATOM   1216  N   GLY A 165       1.363  34.702  10.239  1.00 21.66      A    N
ATOM   1217  CA  GLY A 165       0.537  34.844  11.414  1.00 21.84      A    C
ATOM   1218  C   GLY A 165       0.522  33.581  12.243  1.00 22.27      A    C
ATOM   1219  O   GLY A 165       0.680  32.440  11.713  1.00 22.20      A    O
ATOM   1220  N   SER A 166       0.305  33.762  13.543  1.00 22.06      A    N
ATOM   1221  CA  SER A 166       0.290  32.645  14.470  1.00 21.96      A    C
ATOM   1222  CB  SER A 166       0.344  33.167  15.917  1.00 23.25      A    C
ATOM   1223  OG  SER A 166      -0.948  33.579  16.367  1.00 25.13      A    O
ATOM   1224  C   SER A 166      -0.954  31.807  14.241  1.00 21.45      A    C
ATOM   1225  O   SER A 166      -1.949  32.311  13.716  1.00 21.15      A    O
ATOM   1226  N   GLY A 167      -0.879  30.515  14.574  1.00 20.07      A    N
ATOM   1227  CA  GLY A 167      -2.032  29.639  14.548  1.00 19.63      A    C
ATOM   1228  C   GLY A 167      -2.478  29.248  13.140  1.00 19.18      A    C
ATOM   1229  O   GLY A 167      -3.652  29.051  12.911  1.00 18.57      A    O
ATOM   1230  N   THR A 168      -1.541  29.140  12.200  1.00 18.31      A    N
ATOM   1231  CA  THR A 168      -1.893  28.857  10.810  1.00 17.13      A    C
ATOM   1232  CB  THR A 168      -1.295  29.958   9.908  1.00 17.32      A    C
ATOM   1233  OG1 THR A 168       0.077  30.172  10.261  1.00 14.44      A    O
ATOM   1234  CG2 THR A 168      -1.988  31.299  10.156  1.00 17.60      A    C
ATOM   1235  C   THR A 168      -1.496  27.465  10.306  1.00 16.75      A    C
ATOM   1236  O   THR A 168      -1.462  27.213   9.091  1.00 16.26      A    O
ATOM   1237  N   ILE A 169      -1.265  26.540  11.234  1.00 15.95      A    N
ATOM   1238  CA  ILE A 169      -0.863  25.191  10.871  1.00 15.48      A    C
ATOM   1239  CB  ILE A 169      -0.454  24.378  12.127  1.00 15.09      A    C
ATOM   1240  CG1 ILE A 169       0.626  25.109  12.942  1.00 14.88      A    C
ATOM   1241  CD1 ILE A 169       2.021  25.201  12.267  1.00 16.38      A    C
ATOM   1242  CG2 ILE A 169       0.021  22.988  11.720  1.00 13.45      A    C
ATOM   1243  C   ILE A 169      -2.004  24.477  10.137  1.00 15.22      A    C
ATOM   1244  O   ILE A 169      -3.146  24.470  10.590  1.00 14.50      A    O
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ATOM   1245  N   SER A 170      -1.681  23.857   9.018  1.00 14.94      A    N
ATOM   1246  CA  SER A 170      -2.665  23.060   8.310  1.00 15.41      A    C
ATOM   1247  CB  SER A 170      -2.299  23.004   6.821  1.00 16.02      A    C
ATOM   1248  OG  SER A 170      -1.040  22.404   6.585  1.00 16.03      A    O
ATOM   1249  C   SER A 170      -2.855  21.660   8.904  1.00 15.05      A    C
ATOM   1250  O   SER A 170      -1.986  21.137   9.616  1.00 13.80      A    O
ATOM   1251  N   ALA A 171      -3.992  21.036   8.582  1.00 14.65      A    N
ATOM   1252  CA  ALA A 171      -4.244  19.651   8.933  1.00 14.75      A    C
ATOM   1253  CB  ALA A 171      -5.700  19.507   9.443  1.00 15.62      A    C
ATOM   1254  C   ALA A 171      -4.043  18.750   7.740  1.00 15.02      A    C
ATOM   1255  O   ALA A 171      -4.475  19.096   6.652  1.00 14.12      A    O
ATOM   1256  N   PRO A 172      -3.482  17.548   7.899  1.00 15.48      A    N
ATOM   1257  CA  PRO A 172      -3.078  16.913   9.167  1.00 15.17      A    C
ATOM   1258  CB  PRO A 172      -3.080  15.411   8.796  1.00 15.90      A    C
ATOM   1259  CG  PRO A 172      -3.707  15.336   7.456  1.00 15.73      A    C
ATOM   1260  CD  PRO A 172      -3.401  16.614   6.768  1.00 15.43      A    C
ATOM   1261  C   PRO A 172      -1.724  17.260   9.788  1.00 14.85      A    C
ATOM   1262  O   PRO A 172      -1.284  16.499  10.651  1.00 16.20      A    O
ATOM   1263  N   GLY A 173      -1.086  18.352   9.382  1.00 14.01      A    N
ATOM   1264  CA  GLY A 173       0.078  18.895  10.064  1.00 13.48      A    C
ATOM   1265  C   GLY A 173      -0.158  19.147  11.553  1.00 13.91      A    C
ATOM   1266  O   GLY A 173       0.809  19.174  12.339  1.00 14.08      A    O
ATOM   1267  N   THR A 174      -1.419  19.291  11.956  1.00 13.50      A    N
ATOM   1268  CA  THR A 174      -1.758  19.475  13.375  1.00 13.19      A    C
ATOM   1269  CB  THR A 174      -3.137  20.125  13.530  1.00 13.66      A    C
ATOM   1270  OG1 THR A 174      -4.104  19.394  12.743  1.00 13.16      A    O
ATOM   1271  CG2 THR A 174      -3.114  21.510  12.957  1.00 14.22      A    C
ATOM   1272  C   THR A 174      -1.774  18.188  14.172  1.00 12.85      A    C
ATOM   1273  O   THR A 174      -1.909  18.227  15.390  1.00 12.08      A    O
ATOM   1274  N   ALA A 175      -1.696  17.040  13.505  1.00 12.94      A    N
ATOM   1275  CA  ALA A 175      -1.614  15.772  14.213  1.00 12.90      A    C
ATOM   1276  CB  ALA A 175      -1.422  14.641  13.211  1.00 13.54      A    C
ATOM   1277  C   ALA A 175      -0.484  15.740  15.264  1.00 12.44      A    C
ATOM   1278  O   ALA A 175       0.601  16.233  15.043  1.00 13.06      A    O
ATOM   1279  N   LYS A 176      -0.739  15.131  16.398  1.00 13.08      A    N
ATOM   1280  CA  LYS A 176       0.269  15.057  17.466  1.00 13.00      A    C
ATOM   1281  CB  LYS A 176      -0.383  14.511  18.719  1.00 12.78      A    C
ATOM   1282  CG  LYS A 176      -1.406  15.392  19.366  1.00 13.87      A    C
ATOM   1283  CD  LYS A 176      -2.044  14.693  20.553  1.00 15.77      A    C
ATOM   1284  CE  LYS A 176      -3.179  13.722  20.173  1.00 16.63      A    C
ATOM   1285  NZ  LYS A 176      -3.738  13.048  21.388  1.00 16.58      A    N
ATOM   1286  C   LYS A 176       1.433  14.107  17.115  1.00 13.10      A    C
ATOM   1287  O   LYS A 176       2.559  14.289  17.538  1.00 12.98      A    O
ATOM   1288  N   ASN A 177       1.119  13.047  16.390  1.00 12.81      A    N
ATOM   1289  CA  ASN A 177       2.047  11.933  16.187  1.00 12.78      A    C
ATOM   1290  CB  ASN A 177       1.278  10.628  16.301  1.00 12.48      A    C
ATOM   1291  CG  ASN A 177       0.733  10.382  17.718  1.00 12.12      A    C
ATOM   1292  OD1 ASN A 177       1.135  11.043  18.682  1.00 12.31      A    O
ATOM   1293  ND2 ASN A 177      -0.179   9.416  17.844  1.00 10.81      A    N
ATOM   1294  C   ASN A 177       2.822  11.966  14.876  1.00 12.68      A    C
ATOM   1295  O   ASN A 177       3.692  11.097  14.621  1.00 13.33      A    O
ATOM   1296  N   ALA A 178       2.483  12.933  14.029  1.00 12.80      A    N
ATOM   1297  CA  ALA A 178       3.234  13.208  12.801  1.00 12.70      A    C
ATOM   1298  CB  ALA A 178       2.382  13.938  11.817  1.00 12.83      A    C
ATOM   1299  C   ALA A 178       4.439  14.052  13.141  1.00 12.18      A    C
ATOM   1300  O   ALA A 178       4.471  14.685  14.188  1.00 12.29      A    O
ATOM   1301  N   ILE A 179       5.458  13.985  12.293  1.00 11.71      A    N
ATOM   1302  CA  ILE A 179       6.531  14.966  12.283  1.00 11.72      A    C
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ATOM   1303  CB  ILE A 179       7.838  14.364  11.812  1.00 11.54      A    C
ATOM   1304  CG1 ILE A 179       8.251  13.222  12.712  1.00 13.45      A    C
ATOM   1305  CD1 ILE A 179       9.472  12.467  12.196  1.00 14.82      A    C
ATOM   1306  CG2 ILE A 179       8.927  15.437  11.783  1.00 12.00      A    C
ATOM   1307  C   ILE A 179       6.085  16.076  11.317  1.00 11.98      A    C
ATOM   1308  O   ILE A 179       5.943  15.852  10.109  1.00 11.31      A    O
ATOM   1309  N   THR A 180       5.813  17.248  11.871  1.00 11.27      A    N
ATOM   1310  CA  THR A 180       5.357  18.383  11.074  1.00 11.76      A    C
ATOM   1311  CB  THR A 180       4.260  19.120  11.818  1.00 11.79      A    C
ATOM   1312  OG1 THR A 180       3.166  18.214  12.084  1.00 12.06      A    O
ATOM   1313  CG2 THR A 180       3.603  20.224  10.929  1.00 12.72      A    C
ATOM   1314  C   THR A 180       6.530  19.306  10.690  1.00 11.82      A    C
ATOM   1315  O   THR A 180       7.286  19.762  11.533  1.00 11.02      A    O
ATOM   1316  N   VAL A 181       6.662  19.590   9.401  1.00 11.42      A    N
ATOM   1317  CA  VAL A 181       7.830  20.305   8.899  1.00 11.43      A    C
ATOM   1318  CB  VAL A 181       8.492  19.464   7.814  1.00 11.32      A    C
ATOM   1319  CG1 VAL A 181       9.744  20.118   7.309  1.00 12.42      A    C
ATOM   1320  CG2 VAL A 181       8.757  18.055   8.351  1.00 12.33      A    C
ATOM   1321  C   VAL A 181       7.511  21.680   8.302  1.00 11.62      A    C
ATOM   1322  O   VAL A 181       6.667  21.800   7.399  1.00 12.16      A    O
ATOM   1323  N   GLY A 182       8.187  22.704   8.812  1.00 11.59      A    N
ATOM   1324  CA  GLY A 182       8.095  24.042   8.273  1.00 12.80      A    C
ATOM   1325  C   GLY A 182       9.296  24.352   7.391  1.00 13.72      A    C
ATOM   1326  O   GLY A 182      10.243  23.574   7.344  1.00 14.13      A    O
ATOM   1327  N   ALA A 183       9.264  25.492   6.700  1.00 13.43      A    N
ATOM   1328  CA  ALA A 183      10.312  25.837   5.776  1.00 14.22      A    C
ATOM   1329  CB  ALA A 183       9.709  26.166   4.401  1.00 14.53      A    C
ATOM   1330  C   ALA A 183      11.205  27.001   6.238  1.00 14.32      A    C
ATOM   1331  O   ALA A 183      10.717  28.110   6.498  1.00 14.13      A    O
ATOM   1332  N   THR A 184      12.512  26.737   6.293  1.00 14.17      A    N
ATOM   1333  CA  THR A 184      13.513  27.799   6.294  1.00 14.33      A    C
ATOM   1334  CB  THR A 184      14.743  27.451   7.159  1.00 14.19      A    C
ATOM   1335  OG1 THR A 184      15.180  26.103   6.925  1.00 13.83      A    O
ATOM   1336  CG2 THR A 184      14.383  27.474   8.636  1.00 13.70      A    C
ATOM   1337  C   THR A 184      13.905  28.018   4.841  1.00 15.47      A    C
ATOM   1338  O   THR A 184      13.380  27.354   3.934  1.00 15.87      A    O
ATOM   1339  N   GLU A 185      14.861  28.919   4.618  1.00 15.13      A    N
ATOM   1340  CA  GLU A 185      15.328  29.246   3.290  1.00 14.03      A    C
ATOM   1341  CB  GLU A 185      15.696  30.766   3.230  1.00 13.82      A    C
ATOM   1342  CG  GLU A 185      14.492  31.673   3.495  1.00 15.09      A    C
ATOM   1343  CD  GLU A 185      14.785  33.172   3.329  1.00 14.09      A    C
ATOM   1344  OE1 GLU A 185      15.911  33.541   2.985  1.00 15.60      A    O
ATOM   1345  OE2 GLU A 185      13.871  33.984   3.528  1.00 14.21      A    O
ATOM   1346  C   GLU A 185      16.511  28.376   2.863  1.00 13.70      A    C
ATOM   1347  O   GLU A 185      17.387  28.011   3.675  1.00 14.17      A    O
ATOM   1348  N   ASN A 186      16.521  28.008   1.587  1.00 12.64      A    N
ATOM   1349  CA  ASN A 186      17.707  27.452   0.959  1.00 13.44      A    C
ATOM   1350  CB  ASN A 186      17.345  26.758  -0.353  1.00 13.84      A    C
ATOM   1351  CG  ASN A 186      18.293  25.630  -0.717  1.00 14.82      A    C
ATOM   1352  OD1 ASN A 186      19.084  25.169   0.099  1.00 14.62      A    O
ATOM   1353  ND2 ASN A 186      18.189  25.156  -1.970  1.00 15.51      A    N
ATOM   1354  C   ASN A 186      18.652  28.603   0.681  1.00 13.83      A    C
ATOM   1355  O   ASN A 186      18.244  29.769   0.711  1.00 14.50      A    O
ATOM   1356  N   LEU A 187      19.920  28.298   0.470  1.00 14.83      A    N
ATOM   1357  CA  LEU A 187      20.892  29.352   0.213  1.00 14.62      A    C
ATOM   1358  CB  LEU A 187      22.144  29.144   1.018  1.00 15.48      A    C
ATOM   1359  CG  LEU A 187      23.144  30.319   0.975  1.00 17.25      A    C
ATOM   1360  CD1 LEU A 187      22.504  31.587   1.469  1.00 18.56      A    C
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ATOM   1361  CD2 LEU A 187      24.394  29.973   1.816  1.00 20.46      A    C
ATOM   1362  C   LEU A 187      21.205  29.360  -1.279  1.00 14.80      A    C
ATOM   1363  O   LEU A 187      22.106  28.692  -1.734  1.00 14.07      A    O
ATOM   1364  N   ARG A 188      20.398  30.083  -2.023  1.00 15.63      A    N
ATOM   1365  CA  ARG A 188      20.631  30.308  -3.454  1.00 17.55      A    C
ATOM   1366  CB  ARG A 188      19.658  29.484  -4.273  1.00 17.02      A    C
ATOM   1367  CG  ARG A 188      19.842  27.989  -4.168  1.00 17.82      A    C
ATOM   1368  CD  ARG A 188      19.063  27.213  -5.267  1.00 19.96      A    C
ATOM   1369  NE  ARG A 188      19.315  25.782  -5.224  1.00 18.26      A    N
ATOM   1370  CZ  ARG A 188      20.339  25.172  -5.814  1.00 19.52      A    C
ATOM   1371  NH1 ARG A 188      21.235  25.846  -6.530  1.00 17.91      A    N
ATOM   1372  NH2 ARG A 188      20.475  23.867  -5.693  1.00 19.41      A    N
ATOM   1373  C   ARG A 188      20.387  31.804  -3.694  1.00 17.89      A    C
ATOM   1374  O   ARG A 188      19.379  32.189  -4.251  1.00 18.33      A    O
ATOM   1375  N   PRO A 189      21.273  32.646  -3.181  1.00 19.58      A    N
ATOM   1376  CA  PRO A 189      20.990  34.082  -3.061  1.00 20.68      A    C
ATOM   1377  CB  PRO A 189      22.179  34.613  -2.239  1.00 21.07      A    C
ATOM   1378  CG  PRO A 189      23.271  33.608  -2.417  1.00 21.15      A    C
ATOM   1379  CD  PRO A 189      22.599  32.288  -2.657  1.00 20.12      A    C
ATOM   1380  C   PRO A 189      20.833  34.863  -4.373  1.00 21.39      A    C
ATOM   1381  O   PRO A 189      20.276  35.975  -4.347  1.00 20.51      A    O
ATOM   1382  N   SER A 190      21.285  34.307  -5.492  1.00 22.89      A    N
ATOM   1383  CA  SER A 190      21.033  34.940  -6.796  1.00 24.65      A    C
ATOM   1384  CB  SER A 190      21.685  34.135  -7.932  1.00 24.76      A    C
ATOM   1385  OG  SER A 190      21.082  32.831  -8.046  1.00 25.85      A    O
ATOM   1386  C   SER A 190      19.525  35.098  -7.028  1.00 25.23      A    C
ATOM   1387  O   SER A 190      19.080  35.918  -7.850  1.00 26.47      A    O
ATOM   1388  N   PHE A 191      18.723  34.365  -6.258  1.00 25.36      A    N
ATOM   1389  CA  PHE A 191      17.264  34.446  -6.389  1.00 25.28      A    C
ATOM   1390  CB  PHE A 191      16.643  33.046  -6.156  1.00 25.00      A    C
ATOM   1391  CG  PHE A 191      16.841  32.089  -7.310  1.00 23.34      A    C
ATOM   1392  CD1 PHE A 191      17.565  30.932  -7.159  1.00 21.81      A    C
ATOM   1393  CE1 PHE A 191      17.735  30.052  -8.218  1.00 22.63      A    C
ATOM   1394  CZ  PHE A 191      17.180  30.341  -9.470  1.00 21.46      A    C
ATOM   1395  CE2 PHE A 191      16.449  31.484  -9.631  1.00 22.61      A    C
ATOM   1396  CD2 PHE A 191      16.288  32.361  -8.562  1.00 25.47      A    C
ATOM   1397  C   PHE A 191      16.388  35.561  -5.720  1.00 25.71      A    C
ATOM   1398  O   PHE A 191      15.184  35.500  -5.877  1.00 27.33      A    O
ATOM   1399  N   GLY A 192      16.823  36.552  -4.944  1.00 26.98      A    N
ATOM   1400  CA  GLY A 192      17.639  36.484  -3.783  1.00 26.29      A    C
ATOM   1401  C   GLY A 192      16.795  36.445  -2.478  1.00 25.37      A    C
ATOM   1402  O   GLY A 192      17.008  35.528  -1.733  1.00 25.24      A    O
ATOM   1403  N   SER A 193      15.858  37.355  -2.179  1.00 24.49      A    N
ATOM   1404  CA  SER A 193      15.332  37.444  -0.778  1.00 24.39      A    C
ATOM   1405  CB  SER A 193      14.452  38.689  -0.554  1.00 24.51      A    C
ATOM   1406  OG  SER A 193      13.058  38.407  -0.623  1.00 25.19      A    O
ATOM   1407  C   SER A 193      14.664  36.176  -0.133  1.00 23.94      A    C
ATOM   1408  O   SER A 193      14.740  35.973   1.085  1.00 22.27      A    O
ATOM   1409  N   TYR A 194      14.037  35.331  -0.949  1.00 23.39      A    N
ATOM   1410  CA  TYR A 194      13.497  34.046  -0.477  1.00 23.08      A    C
ATOM   1411  CB  TYR A 194      12.407  33.559  -1.439  1.00 23.87      A    C
ATOM   1412  CG  TYR A 194      11.044  34.129  -1.144  1.00 27.80      A    C
ATOM   1413  CD1 TYR A 194      10.563  35.240  -1.832  1.00 31.12      A    C
ATOM   1414  CE1 TYR A 194       9.317  35.775  -1.554  1.00 32.91      A    C
ATOM   1415  CZ  TYR A 194       8.525  35.182  -0.591  1.00 34.12      A    C
ATOM   1416  OH  TYR A 194       7.282  35.696  -0.311  1.00 38.22      A    O
ATOM   1417  CE2 TYR A 194       8.974  34.076   0.108  1.00 33.28      A    C
ATOM   1418  CD2 TYR A 194      10.229  33.556  -0.169  1.00 31.26      A    C
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ATOM   1419  C   TYR A 194      14.545  32.930  -0.289  1.00 21.59      A    C
ATOM   1420  O   TYR A 194      14.225  31.848   0.236  1.00 20.33      A    O
ATOM   1421  N   ALA A 195      15.785  33.185  -0.695  1.00 20.44      A    N
ATOM   1422  CA  ALA A 195      16.838  32.181  -0.610  1.00 20.47      A    C
ATOM   1423  CB  ALA A 195      16.915  31.365  -1.892  1.00 20.41      A    C
ATOM   1424  C   ALA A 195      18.222  32.757  -0.270  1.00 19.93      A    C
ATOM   1425  O   ALA A 195      19.230  32.354  -0.877  1.00 19.21      A    O
ATOM   1426  N   ASP A 196      18.264  33.615   0.750  1.00 19.15      A    N
ATOM   1427  CA  ASP A 196      19.472  34.355   1.126  1.00 19.86      A    C
ATOM   1428  CB  ASP A 196      19.264  35.861   0.919  1.00 20.04      A    C
ATOM   1429  CG  ASP A 196      18.198  36.453   1.814  1.00 22.11      A    C
ATOM   1430  OD1 ASP A 196      18.040  37.693   1.696  1.00 23.87      A    O
ATOM   1431  OD2 ASP A 196      17.461  35.822   2.649  1.00 19.55      A    O
ATOM   1432  C   ASP A 196      20.025  34.163   2.549  1.00 19.90      A    C
ATOM   1433  O   ASP A 196      21.092  34.705   2.869  1.00 19.61      A    O
ATOM   1434  N   ASN A 197      19.326  33.410   3.394  1.00 18.85      A    N
ATOM   1435  CA  ASN A 197      19.790  33.177   4.757  1.00 18.29      A    C
ATOM   1436  CB  ASN A 197      19.410  34.369   5.644  1.00 18.68      A    C
ATOM   1437  CG  ASN A 197      20.123  34.360   7.001  1.00 19.48      A    C
ATOM   1438  OD1 ASN A 197      20.221  33.319   7.630  1.00 16.60      A    O
ATOM   1439  ND2 ASN A 197      20.603  35.541   7.455  1.00 14.55      A    N
ATOM   1440  C   ASN A 197      19.198  31.861   5.304  1.00 17.30      A    C
ATOM   1441  O   ASN A 197      17.986  31.734   5.463  1.00 16.96      A    O
ATOM   1442  N   ILE A 198      20.066  30.901   5.608  1.00 16.67      A    N
ATOM   1443  CA  ILE A 198      19.606  29.557   5.993  1.00 16.04      A    C
ATOM   1444  CB  ILE A 198      20.771  28.571   6.020  1.00 15.64      A    C
ATOM   1445  CG1 ILE A 198      21.724  28.885   7.179  1.00 16.27      A    C
ATOM   1446  CD1 ILE A 198      22.734  27.781   7.490  1.00 18.08      A    C
ATOM   1447  CG2 ILE A 198      21.459  28.530   4.679  1.00 16.50      A    C
ATOM   1448  C   ILE A 198      18.897  29.560   7.352  1.00 15.03      A    C
ATOM   1449  O   ILE A 198      18.222  28.605   7.723  1.00 15.12      A    O
ATOM   1450  N   ASN A 199      19.054  30.642   8.102  1.00 14.78      A    N
ATOM   1451  CA  ASN A 199      18.316  30.794   9.344  1.00 14.68      A    C
ATOM   1452  CB  ASN A 199      19.180  31.609  10.332  1.00 14.98      A    C
ATOM   1453  CG  ASN A 199      20.487  30.948  10.708  1.00 15.69      A    C
ATOM   1454  OD1 ASN A 199      20.560  29.757  10.907  1.00 14.98      A    O
ATOM   1455  ND2 ASN A 199      21.526  31.768  10.903  1.00 20.04      A    N
ATOM   1456  C   ASN A 199      17.036  31.597   9.311  1.00 14.49      A    C
ATOM   1457  O   ASN A 199      16.239  31.490  10.227  1.00 14.69      A    O
ATOM   1458  N   HIS A 200      16.736  32.328   8.241  1.00 15.73      A    N
ATOM   1459  CA  HIS A 200      15.375  32.648   7.854  1.00 14.99      A    C
ATOM   1460  CB  HIS A 200      15.338  33.612   6.641  1.00 15.17      A    C
ATOM   1461  CG  HIS A 200      16.005  34.942   6.871  1.00 17.24      A    C
ATOM   1462  ND1 HIS A 200      16.242  35.840   5.842  1.00 16.94      A    N
ATOM   1463  CE1 HIS A 200      16.842  36.916   6.327  1.00 19.73      A    C
ATOM   1464  NE2 HIS A 200      17.009  36.751   7.628  1.00 17.79      A    N
ATOM   1465  CD2 HIS A 200      16.469  35.538   7.999  1.00 18.37      A    C
ATOM   1466  C   HIS A 200      14.327  31.581   7.730  1.00 15.01      A    C
ATOM   1467  O   HIS A 200      14.472  30.673   6.965  1.00 14.41      A    O
ATOM   1468  N   VAL A 201      13.251  31.772   8.496  1.00 15.72      A    N
ATOM   1469  CA  VAL A 201      12.004  31.059   8.294  1.00 16.37      A    C
ATOM   1470  CB  VAL A 201      11.103  31.185   9.523  1.00 16.41      A    C
ATOM   1471  CG1 VAL A 201       9.780  30.428   9.297  1.00 16.12      A    C
ATOM   1472  CG2 VAL A 201      11.841  30.668  10.783  1.00 18.01      A    C
ATOM   1473  C   VAL A 201      11.313  31.683   7.089  1.00 16.94      A    C
ATOM   1474  O   VAL A 201      11.250  32.900   6.973  1.00 17.09      A    O
ATOM   1475  N   ALA A 202      10.872  30.865   6.143  1.00 17.70      A    N
ATOM   1476  CA  ALA A 202      10.233  31.396   4.949  1.00 17.52      A    C
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ATOM	1477	CB	ALA	A	202	9.859	30.265	4.018	1.00	18.76	A	C
ATOM	1478	C	ALA	A	202	9.000	32.169	5.383	1.00	17.84	A	C
ATOM	1479	O	ALA	A	202	8.263	31.734	6.263	1.00	16.60	A	O
ATOM	1480	N	GLN	A	203	8.770	33.332	4.783	1.00	18.20	A	N
ATOM	1481	CA	GLN	A	203	7.629	34.135	5.192	1.00	19.45	A	C
ATOM	1482	CB	BGLN	A	203	7.542	35.347	4.260	0.40	19.94	A	C
ATOM	1483	CB	AGLN	A	203	7.529	35.467	4.445	0.60	20.39	A	C
ATOM	1484	CG	BGLN	A	203	7.527	36.681	4.943	0.40	22.36	A	C
ATOM	1485	CG	AGLN	A	203	6.748	36.514	5.261	0.60	24.58	A	C
ATOM	1486	CD	BGLN	A	203	6.379	37.556	4.452	0.40	25.52	A	C
ATOM	1487	CD	AGLN	A	203	7.553	37.090	6.439	0.60	28.39	A	C
ATOM	1488	OE1	BGLN	A	203	5.568	37.122	3.624	0.40	27.97	A	O
ATOM	1489	OE1	AGLN	A	203	8.525	37.816	6.236	0.60	33.69	A	O
ATOM	1490	NE2	BGLN	A	203	6.299	38.772	4.972	0.40	24.61	A	N
ATOM	1491	NE2	AGLN	A	203	7.155	36.751	7.655	0.60	31.16	A	N
ATOM	1492	C	GLN	A	203	6.291	33.391	5.152	1.00	18.58	A	C
ATOM	1493	O	GLN	A	203	5.458	33.580	6.028	1.00	18.67	A	O
ATOM	1494	N	PHE	A	204	6.090	32.533	4.163	1.00	17.22	A	N
ATOM	1495	CA	PHE	A	204	4.805	31.833	4.027	1.00	16.75	A	C
ATOM	1496	CB	PHE	A	204	4.603	31.335	2.589	1.00	16.25	A	C
ATOM	1497	CG	PHE	A	204	5.720	30.475	2.093	1.00	16.52	A	C
ATOM	1498	CD1	PHE	A	204	5.857	29.158	2.526	1.00	16.66	A	C
ATOM	1499	CE1	PHE	A	204	6.893	28.378	2.083	1.00	17.13	A	C
ATOM	1500	CZ	PHE	A	204	7.854	28.909	1.234	1.00	14.67	A	C
ATOM	1501	CE2	PHE	A	204	7.747	30.231	0.816	1.00	16.10	A	C
ATOM	1502	CD2	PHE	A	204	6.693	31.009	1.267	1.00	15.39	A	C
ATOM	1503	C	PHE	A	204	4.670	30.647	5.018	1.00	16.21	A	C
ATOM	1504	O	PHE	A	204	3.570	30.150	5.198	1.00	15.42	A	O
ATOM	1505	N	SER	A	205	5.754	30.223	5.688	1.00	15.36	A	N
ATOM	1506	CA	SER	A	205	5.692	28.983	6.508	1.00	15.18	A	C
ATOM	1507	CB	SER	A	205	7.068	28.579	7.063	1.00	15.27	A	C
ATOM	1508	OG	SER	A	205	7.042	27.254	7.585	1.00	15.10	A	O
ATOM	1509	C	SER	A	205	4.657	29.103	7.615	1.00	14.84	A	C
ATOM	1510	O	SER	A	205	4.618	30.092	8.319	1.00	16.26	A	O
ATOM	1511	N	SER	A	206	3.764	28.141	7.753	1.00	15.82	A	N
ATOM	1512	CA	SER	A	206	2.751	28.237	8.818	1.00	15.73	A	C
ATOM	1513	CB	SER	A	206	1.714	27.117	8.735	1.00	16.10	A	C
ATOM	1514	OG	SER	A	206	0.811	27.350	7.655	1.00	14.83	A	O
ATOM	1515	C	SER	A	206	3.421	28.221	10.186	1.00	15.92	A	C
ATOM	1516	O	SER	A	206	4.486	27.589	10.362	1.00	15.30	A	O
ATOM	1517	N	ARG	A	207	2.786	28.928	11.113	1.00	15.72	A	N
ATOM	1518	CA	ARG	A	207	3.289	29.140	12.455	1.00	16.34	A	C
ATOM	1519	CB	ARG	A	207	3.511	30.636	12.715	1.00	16.50	A	C
ATOM	1520	CG	ARG	A	207	4.189	31.375	11.542	1.00	18.52	A	C
ATOM	1521	CD	ARG	A	207	5.604	30.916	11.227	1.00	20.29	A	C
ATOM	1522	NE	ARG	A	207	6.146	31.519	10.012	1.00	22.13	A	N
ATOM	1523	CZ	ARG	A	207	6.821	32.643	9.981	1.00	22.20	A	C
ATOM	1524	NH1	ARG	A	207	7.056	33.294	11.080	1.00	25.41	A	N
ATOM	1525	NH2	ARG	A	207	7.256	33.124	8.838	1.00	24.08	A	N
ATOM	1526	C	ARG	A	207	2.330	28.556	13.471	1.00	15.97	A	C
ATOM	1527	O	ARG	A	207	1.096	28.605	13.301	1.00	15.01	A	O
ATOM	1528	N	GLY	A	208	2.903	27.974	14.521	1.00	15.16	A	N
ATOM	1529	CA	GLY	A	208	2.139	27.523	15.655	1.00	16.14	A	C
ATOM	1530	C	GLY	A	208	1.622	28.688	16.476	1.00	16.50	A	C
ATOM	1531	O	GLY	A	208	1.753	29.830	16.059	1.00	17.36	A	O
ATOM	1532	N	PRO	A	209	0.999	28.423	17.617	1.00	17.42	A	N
ATOM	1533	CA	PRO	A	209	0.727	27.067	18.089	1.00	17.56	A	C
ATOM	1534	CB	PRO	A	209	0.407	27.269	19.579	1.00	17.58	A	C

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ATOM   1535  CG  PRO A 209      -0.088  28.644  19.701  1.00 18.85      A    C
ATOM   1536  CD  PRO A 209       0.477  29.457  18.545  1.00 17.85      A    C
ATOM   1537  C   PRO A 209      -0.483  26.483  17.368  1.00 17.50      A    C
ATOM   1538  O   PRO A 209      -1.094  27.157  16.558  1.00 18.18      A    O
ATOM   1539  N   THR A 210      -0.816  25.240  17.652  1.00 16.70      A    N
ATOM   1540  CA  THR A 210      -2.050  24.690  17.186  1.00 17.34      A    C
ATOM   1541  CB  THR A 210      -2.042  23.181  17.356  1.00 16.73      A    C
ATOM   1542  OG1 THR A 210      -1.848  22.859  18.734  1.00 18.34      A    O
ATOM   1543  CG2 THR A 210      -0.833  22.540  16.574  1.00 16.90      A    C
ATOM   1544  C   THR A 210      -3.206  25.327  17.987  1.00 17.55      A    C
ATOM   1545  O   THR A 210      -2.990  26.095  18.930  1.00 16.40      A    O
ATOM   1546  N   ARG A 211      -4.421  24.979  17.623  1.00 18.89      A    N
ATOM   1547  CA  ARG A 211      -5.595  25.577  18.264  1.00 20.56      A    C
ATOM   1548  CB  ARG A 211      -6.884  25.056  17.638  1.00 21.16      A    C
ATOM   1549  CG  ARG A 211      -8.149  25.719  18.255  1.00 25.92      A    C
ATOM   1550  CD  ARG A 211      -9.325  25.804  17.301  1.00 31.08      A    C
ATOM   1551  NE  ARG A 211      -8.956  26.457  16.042  1.00 35.63      A    N
ATOM   1552  CZ  ARG A 211      -9.626  26.296  14.905  1.00 38.91      A    C
ATOM   1553  NH1 ARG A 211     -10.707  25.516  14.876  1.00 40.64      A    N
ATOM   1554  NH2 ARG A 211      -9.225  26.911  13.795  1.00 37.74      A    N
ATOM   1555  C   ARG A 211      -5.591  25.308  19.768  1.00 20.16      A    C
ATOM   1556  O   ARG A 211      -5.983  26.180  20.539  1.00 19.93      A    O
ATOM   1557  N   ASP A 212      -5.120  24.121  20.185  1.00 19.40      A    N
ATOM   1558  CA  ASP A 212      -5.031  23.791  21.616  1.00 18.64      A    C
ATOM   1559  CB  ASP A 212      -5.346  22.306  21.877  1.00 18.58      A    C
ATOM   1560  CG  ASP A 212      -4.318  21.356  21.254  1.00 16.59      A    C
ATOM   1561  OD1 ASP A 212      -4.255  20.180  21.679  1.00 16.40      A    O
ATOM   1562  OD2 ASP A 212      -3.545  21.688  20.339  1.00 17.56      A    O
ATOM   1563  C   ASP A 212      -3.693  24.160  22.255  1.00 18.83      A    C
ATOM   1564  O   ASP A 212      -3.387  23.707  23.370  1.00 19.22      A    O
ATOM   1565  N   GLY A 213      -2.902  24.966  21.556  1.00 18.29      A    N
ATOM   1566  CA  GLY A 213      -1.698  25.572  22.111  1.00 18.10      A    C
ATOM   1567  C   GLY A 213      -0.439  24.713  22.065  1.00 17.75      A    C
ATOM   1568  O   GLY A 213       0.517  24.998  22.785  1.00 18.06      A    O
ATOM   1569  N   ARG A 214      -0.431  23.665  21.242  1.00 16.43      A    N
ATOM   1570  CA  ARG A 214       0.757  22.826  21.110  1.00 16.72      A    C
ATOM   1571  CB  ARG A 214       0.403  21.461  20.536  1.00 16.17      A    C
ATOM   1572  CG  ARG A 214      -0.276  20.553  21.473  1.00 16.40      A    C
ATOM   1573  CD  ARG A 214      -0.753  19.301  20.814  1.00 16.61      A    C
ATOM   1574  NE  ARG A 214      -1.771  19.613  19.826  1.00 16.67      A    N
ATOM   1575  CZ  ARG A 214      -1.740  19.297  18.531  1.00 16.71      A    C
ATOM   1576  NH1 ARG A 214      -0.720  18.628  17.981  1.00 16.55      A    N
ATOM   1577  NH2 ARG A 214      -2.762  19.664  17.776  1.00 14.42      A    N
ATOM   1578  C   ARG A 214       1.772  23.493  20.203  1.00 16.16      A    C
ATOM   1579  O   ARG A 214       1.403  24.306  19.344  1.00 16.86      A    O
ATOM   1580  N   ILE A 215       3.046  23.168  20.396  1.00 15.82      A    N
ATOM   1581  CA  ILE A 215       4.107  23.640  19.516  1.00 15.40      A    C
ATOM   1582  CB  ILE A 215       5.503  23.498  20.175  1.00 16.18      A    C
ATOM   1583  CG1 ILE A 215       5.600  24.351  21.454  1.00 17.35      A    C
ATOM   1584  CD1 ILE A 215       5.526  25.842  21.181  1.00 20.01      A    C
ATOM   1585  CG2 ILE A 215       6.606  23.898  19.191  1.00 15.87      A    C
ATOM   1586  C   ILE A 215       4.100  22.834  18.214  1.00 15.40      A    C
ATOM   1587  O   ILE A 215       4.316  21.616  18.227  1.00 14.96      A    O
ATOM   1588  N   LYS A 216       3.841  23.536  17.117  1.00 14.61      A    N
ATOM   1589  CA  LYS A 216       4.072  23.062  15.745  1.00 14.64      A    C
ATOM   1590  CB  LYS A 216       2.765  22.616  15.067  1.00 13.98      A    C
ATOM   1591  CG  LYS A 216       2.190  21.271  15.526  1.00 13.46      A    C
ATOM   1592  CD  LYS A 216       3.073  20.102  15.117  1.00 14.36      A    C
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ATOM	1593	CE	LYS	A	216	2.427	18.754	15.453	1.00	13.24	A	C
ATOM	1594	NZ	LYS	A	216	3.042	17.577	14.739	1.00	8.08	A	N
ATOM	1595	C	LYS	A	216	4.632	24.269	14.984	1.00	14.70	A	C
ATOM	1596	O	LYS	A	216	4.336	25.428	15.358	1.00	13.92	A	O
ATOM	1597	N	PRO	A	217	5.410	24.032	13.921	1.00	14.59	A	N
ATOM	1598	CA	PRO	A	217	5.788	22.691	13.468	1.00	13.65	A	C
ATOM	1599	CB	PRO	A	217	6.452	22.944	12.115	1.00	14.58	A	C
ATOM	1600	CG	PRO	A	217	6.934	24.356	12.178	1.00	15.23	A	C
ATOM	1601	CD	PRO	A	217	6.012	25.077	13.086	1.00	14.44	A	C
ATOM	1602	C	PRO	A	217	6.818	22.089	14.401	1.00	12.99	A	C
ATOM	1603	O	PRO	A	217	7.262	22.738	15.379	1.00	12.11	A	O
ATOM	1604	N	ASP	A	218	7.201	20.847	14.126	1.00	11.74	A	N
ATOM	1605	CA	ASP	A	218	8.188	20.214	14.974	1.00	11.35	A	C
ATOM	1606	CB	ASP	A	218	8.033	18.694	14.962	1.00	11.47	A	C
ATOM	1607	CG	ASP	A	218	6.672	18.241	15.451	1.00	11.82	A	C
ATOM	1608	OD1	ASP	A	218	6.440	18.370	16.680	1.00	10.57	A	O
ATOM	1609	OD2	ASP	A	218	5.810	17.726	14.671	1.00	11.50	A	O
ATOM	1610	C	ASP	A	218	9.619	20.566	14.610	1.00	11.30	A	C
ATOM	1611	O	ASP	A	218	10.441	20.772	15.501	1.00	10.85	A	O
ATOM	1612	N	VAL	A	219	9.928	20.516	13.314	1.00	11.61	A	N
ATOM	1613	CA	VAL	A	219	11.254	20.829	12.815	1.00	12.37	A	C
ATOM	1614	CB	VAL	A	219	12.118	19.589	12.602	1.00	12.19	A	C
ATOM	1615	CG1	VAL	A	219	12.401	18.867	13.933	1.00	14.24	A	C
ATOM	1616	CG2	VAL	A	219	11.485	18.660	11.587	1.00	13.54	A	C
ATOM	1617	C	VAL	A	219	11.148	21.568	11.471	1.00	12.33	A	C
ATOM	1618	O	VAL	A	219	10.083	21.624	10.851	1.00	12.34	A	O
ATOM	1619	N	MET	A	220	12.266	22.139	11.057	1.00	11.78	A	N
ATOM	1620	CA	MET	A	220	12.365	22.930	9.852	1.00	11.89	A	C
ATOM	1621	CB	MET	A	220	12.798	24.371	10.167	1.00	11.30	A	C
ATOM	1622	CG	MET	A	220	12.025	25.058	11.255	1.00	11.64	A	C
ATOM	1623	SD	MET	A	220	10.310	25.322	10.860	1.00	12.02	A	S
ATOM	1624	CE	MET	A	220	10.416	26.727	9.791	1.00	11.35	A	C
ATOM	1625	C	MET	A	220	13.398	22.343	8.902	1.00	12.21	A	C
ATOM	1626	O	MET	A	220	14.368	21.731	9.321	1.00	12.24	A	O
ATOM	1627	N	ALA	A	221	13.175	22.556	7.613	1.00	12.60	A	N
ATOM	1628	CA	ALA	A	221	14.198	22.324	6.605	1.00	12.90	A	C
ATOM	1629	CB	ALA	A	221	14.098	20.912	6.081	1.00	12.23	A	C
ATOM	1630	C	ALA	A	221	14.064	23.341	5.464	1.00	13.77	A	C
ATOM	1631	O	ALA	A	221	13.029	24.027	5.312	1.00	14.46	A	O
ATOM	1632	N	PRO	A	222	15.116	23.487	4.687	1.00	13.99	A	N
ATOM	1633	CA	PRO	A	222	15.059	24.393	3.543	1.00	14.73	A	C
ATOM	1634	CB	PRO	A	222	16.387	24.159	2.845	1.00	13.69	A	C
ATOM	1635	CG	PRO	A	222	17.290	23.676	3.892	1.00	15.06	A	C
ATOM	1636	CD	PRO	A	222	16.433	22.855	4.830	1.00	14.39	A	C
ATOM	1637	C	PRO	A	222	13.896	24.044	2.622	1.00	14.82	A	C
ATOM	1638	O	PRO	A	222	13.719	22.847	2.284	1.00	15.21	A	O
ATOM	1639	N	GLY	A	223	13.178	25.069	2.193	1.00	14.57	A	N
ATOM	1640	CA	GLY	A	223	11.996	24.910	1.373	1.00	15.06	A	C
ATOM	1641	C	GLY	A	223	11.779	26.046	0.383	1.00	14.81	A	C
ATOM	1642	O	GLY	A	223	10.661	26.268	-0.039	1.00	15.67	A	O
ATOM	1643	N	THR	A	224	12.822	26.799	0.049	1.00	13.98	A	N
ATOM	1644	CA	THR	A	224	12.706	27.772	-1.007	1.00	14.01	A	C
ATOM	1645	CB	THR	A	224	12.912	29.229	-0.517	1.00	13.98	A	C
ATOM	1646	OG1	THR	A	224	14.220	29.350	0.047	1.00	13.39	A	O
ATOM	1647	CG2	THR	A	224	11.952	29.585	0.597	1.00	14.59	A	C
ATOM	1648	C	THR	A	224	13.729	27.449	-2.072	1.00	14.02	A	C
ATOM	1649	O	THR	A	224	14.813	26.932	-1.791	1.00	14.13	A	O
ATOM	1650	N	TYR	A	225	13.389	27.786	-3.308	1.00	14.73	A	N

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ATOM   1651  CA  TYR A 225      14.270  27.528  -4.441  1.00 14.78      A    C
ATOM   1652  CB  TYR A 225      15.197  28.726  -4.686  1.00 15.26      A    C
ATOM   1653  CG  TYR A 225      14.502  29.848  -5.398  1.00 15.90      A    C
ATOM   1654  CD1 TYR A 225      14.027  30.940  -4.692  1.00 18.12      A    C
ATOM   1655  CE1 TYR A 225      13.349  31.960  -5.301  1.00 18.57      A    C
ATOM   1656  CZ  TYR A 225      13.100  31.918  -6.659  1.00 19.46      A    C
ATOM   1657  OH  TYR A 225      12.391  32.974  -7.207  1.00 20.70      A    O
ATOM   1658  CE2 TYR A 225      13.510  30.844  -7.404  1.00 18.30      A    C
ATOM   1659  CD2 TYR A 225      14.225  29.788  -6.771  1.00 19.15      A    C
ATOM   1660  C   TYR A 225      15.022  26.196  -4.331  1.00 14.79      A    C
ATOM   1661  O   TYR A 225      16.252  26.119  -4.395  1.00 15.52      A    O
ATOM   1662  N   ILE A 226      14.248  25.130  -4.186  1.00 15.07      A    N
ATOM   1663  CA  ILE A 226      14.773  23.759  -4.155  1.00 14.45      A    C
ATOM   1664  CB  ILE A 226      13.904  22.866  -3.254  1.00 14.35      A    C
ATOM   1665  CG1 ILE A 226      13.906  23.341  -1.789  1.00 15.47      A    C
ATOM   1666  CD1 ILE A 226      15.239  23.250  -1.085  1.00 16.51      A    C
ATOM   1667  CG2 ILE A 226      14.312  21.400  -3.377  1.00 14.04      A    C
ATOM   1668  C   ILE A 226      14.780  23.205  -5.580  1.00 14.24      A    C
ATOM   1669  O   ILE A 226      13.778  23.188  -6.245  1.00 13.78      A    O
ATOM   1670  N   LEU A 227      15.937  22.753  -6.022  1.00 14.94      A    N
ATOM   1671  CA  LEU A 227      16.141  22.230  -7.359  1.00 14.97      A    C
ATOM   1672  CB  LEU A 227      17.541  22.653  -7.827  1.00 15.61      A    C
ATOM   1673  CG  LEU A 227      17.950  22.137  -9.196  1.00 16.60      A    C
ATOM   1674  CD1 LEU A 227      16.899  22.508 -10.231  1.00 16.90      A    C
ATOM   1675  CD2 LEU A 227      19.340  22.669  -9.559  1.00 18.98      A    C
ATOM   1676  C   LEU A 227      16.010  20.708  -7.284  1.00 14.76      A    C
ATOM   1677  O   LEU A 227      16.803  20.038  -6.602  1.00 15.34      A    O
ATOM   1678  N   SER A 228      14.970  20.179  -7.924  1.00 14.03      A    N
ATOM   1679  CA  SER A 228      14.665  18.752  -7.871  1.00 14.07      A    C
ATOM   1680  CB  SER A 228      13.701  18.448  -6.701  1.00 13.81      A    C
ATOM   1681  OG  SER A 228      13.631  17.038  -6.453  1.00 12.38      A    O
ATOM   1682  C   SER A 228      14.061  18.319  -9.208  1.00 14.98      A    C
ATOM   1683  O   SER A 228      13.971  19.115 -10.133  1.00 15.43      A    O
ATOM   1684  N   ALA A 229      13.626  17.067  -9.278  1.00 14.57      A    N
ATOM   1685  CA  ALA A 229      13.155  16.454 -10.516  1.00 14.87      A    C
ATOM   1686  CB  ALA A 229      12.824  14.945 -10.268  1.00 14.78      A    C
ATOM   1687  C   ALA A 229      11.939  17.135 -11.086  1.00 14.83      A    C
ATOM   1688  O   ALA A 229      10.939  17.411 -10.376  1.00 14.22      A    O
ATOM   1689  N   ARG A 230      12.027  17.381 -12.394  1.00 14.42      A    N
ATOM   1690  CA  ARG A 230      10.974  18.013 -13.155  1.00 14.49      A    C
ATOM   1691  CB  ARG A 230      11.553  19.008 -14.137  1.00 14.60      A    C
ATOM   1692  CG  ARG A 230      10.516  19.626 -15.065  1.00 16.55      A    C
ATOM   1693  CD  ARG A 230      11.044  20.792 -15.934  1.00 19.98      A    C
ATOM   1694  NE  ARG A 230       9.940  21.308 -16.751  1.00 19.63      A    N
ATOM   1695  CZ  ARG A 230       9.692  22.581 -16.995  1.00 21.34      A    C
ATOM   1696  NH1 ARG A 230      10.502  23.547 -16.545  1.00 21.55      A    N
ATOM   1697  NH2 ARG A 230       8.617  22.898 -17.730  1.00 20.71      A    N
ATOM   1698  C   ARG A 230      10.232  16.947 -13.948  1.00 14.81      A    C
ATOM   1699  O   ARG A 230      10.838  16.237 -14.762  1.00 14.40      A    O
ATOM   1700  N   SER A 231       8.931  16.837 -13.703  1.00 14.68      A    N
ATOM   1701  CA  SER A 231       8.106  15.937 -14.463  1.00 15.32      A    C
ATOM   1702  CB  SER A 231       6.660  16.034 -14.030  1.00 15.75      A    C
ATOM   1703  OG  SER A 231       5.836  15.317 -14.947  1.00 16.08      A    O
ATOM   1704  C   SER A 231       8.176  16.325 -15.956  1.00 15.44      A    C
ATOM   1705  O   SER A 231       8.087  17.494 -16.306  1.00 13.31      A    O
ATOM   1706  N   SER A 232       8.295  15.321 -16.802  1.00 15.69      A    N
ATOM   1707  CA  SER A 232       8.323  15.494 -18.255  1.00 16.52      A    C
ATOM   1708  CB  SER A 232       8.682  14.156 -18.906  1.00 16.29      A    C
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ATOM   1709  OG  SER A 232       7.610  13.191 -18.730  1.00 16.72      A    O
ATOM   1710  C   SER A 232       7.004  16.050 -18.820  1.00 18.10      A    C
ATOM   1711  O   SER A 232       6.970  16.540 -19.945  1.00 18.08      A    O
ATOM   1712  N   LEU A 233       5.924  16.005 -18.040  1.00 18.99      A    N
ATOM   1713  CA  LEU A 233       4.647  16.550 -18.466  1.00 19.87      A    C
ATOM   1714  CB  LEU A 233       3.503  15.655 -17.989  1.00 20.52      A    C
ATOM   1715  CG  LEU A 233       3.579  14.202 -18.428  1.00 22.45      A    C
ATOM   1716  CD1 LEU A 233       2.344  13.472 -17.943  1.00 25.84      A    C
ATOM   1717  CD2 LEU A 233       3.683  14.146 -19.948  1.00 26.24      A    C
ATOM   1718  C   LEU A 233       4.357  17.956 -17.940  1.00 20.22      A    C
ATOM   1719  O   LEU A 233       3.365  18.546 -18.345  1.00 20.30      A    O
ATOM   1720  N   ALA A 234       5.164  18.485 -17.016  1.00 18.84      A    N
ATOM   1721  CA  ALA A 234       4.768  19.731 -16.365  1.00 19.34      A    C
ATOM   1722  CB  ALA A 234       5.297  19.781 -14.958  1.00 18.58      A    C
ATOM   1723  C   ALA A 234       5.197  20.991 -17.153  1.00 19.93      A    C
ATOM   1724  O   ALA A 234       6.300  21.037 -17.701  1.00 20.41      A    O
ATOM   1725  N   PRO A 235       4.325  21.989 -17.197  1.00 20.75      A    N
ATOM   1726  CA  PRO A 235       4.642  23.288 -17.802  1.00 21.88      A    C
ATOM   1727  CB  PRO A 235       3.271  23.921 -17.981  1.00 21.83      A    C
ATOM   1728  CG  PRO A 235       2.429  23.326 -16.902  1.00 21.93      A    C
ATOM   1729  CD  PRO A 235       2.947  21.944 -16.677  1.00 21.22      A    C
ATOM   1730  C   PRO A 235       5.495  24.199 -16.885  1.00 22.70      A    C
ATOM   1731  O   PRO A 235       5.513  23.970 -15.671  1.00 21.06      A    O
ATOM   1732  N   ASP A 236       6.150  25.204 -17.489  1.00 24.00      A    N
ATOM   1733  CA  ASP A 236       6.960  26.228 -16.795  1.00 24.41      A    C
ATOM   1734  CB  ASP A 236       7.455  27.332 -17.750  1.00 24.21      A    C
ATOM   1735  CG  ASP A 236       8.603  26.838 -18.636  1.00 25.42      A    C
ATOM   1736  OD1 ASP A 236       9.214  27.656 -19.365  1.00 25.18      A    O
ATOM   1737  OD2 ASP A 236       8.990  25.634 -18.674  1.00 23.87      A    O
ATOM   1738  C   ASP A 236       6.263  26.644 -15.520  1.00 24.33      A    C
ATOM   1739  O   ASP A 236       6.919  27.035 -14.558  1.00 24.16      A    O
ATOM   1740  N   SER A 237       4.933  26.677 -15.491  1.00 25.32      A    N
ATOM   1741  CA  SER A 237       4.179  27.723 -14.873  1.00 24.89      A    C
ATOM   1742  CB  SER A 237       2.801  27.926 -15.490  1.00 25.98      A    C
ATOM   1743  OG  SER A 237       2.035  26.723 -15.436  1.00 27.95      A    O
ATOM   1744  C   SER A 237       4.027  26.960 -13.487  1.00 24.14      A    C
ATOM   1745  O   SER A 237       3.588  27.516 -12.495  1.00 23.01      A    O
ATOM   1746  N   SER A 238       4.363  25.660 -13.448  1.00 22.59      A    N
ATOM   1747  CA  SER A 238       4.313  24.861 -12.201  1.00 22.41      A    C
ATOM   1748  CB  SER A 238       4.238  23.344 -12.501  1.00 22.11      A    C
ATOM   1749  OG  SER A 238       3.046  22.968 -13.146  1.00 22.38      A    O
ATOM   1750  C   SER A 238       5.543  25.045 -11.295  1.00 21.86      A    C
ATOM   1751  O   SER A 238       5.550  24.542 -10.184  1.00 22.29      A    O
ATOM   1752  N   PHE A 239       6.568  25.744 -11.789  1.00 21.32      A    N
ATOM   1753  CA  PHE A 239       7.847  25.899 -11.108  1.00 20.67      A    C
ATOM   1754  CB  PHE A 239       8.966  25.299 -11.966  1.00 20.17      A    C
ATOM   1755  CG  PHE A 239       8.736  23.854 -12.294  1.00 20.18      A    C
ATOM   1756  CD1 PHE A 239       8.964  22.881 -11.344  1.00 18.34      A    C
ATOM   1757  CE1 PHE A 239       8.686  21.573 -11.600  1.00 15.67      A    C
ATOM   1758  CZ  PHE A 239       8.194  21.184 -12.814  1.00 16.81      A    C
ATOM   1759  CE2 PHE A 239       7.924  22.128 -13.775  1.00 16.81      A    C
ATOM   1760  CD2 PHE A 239       8.194  23.466 -13.520  1.00 18.63      A    C
ATOM   1761  C   PHE A 239       8.124  27.370 -10.775  1.00 20.81      A    C
ATOM   1762  O   PHE A 239       7.589  28.283 -11.404  1.00 19.94      A    O
ATOM   1763  N   TRP A 240       8.927  27.575  -9.743  1.00 20.46      A    N
ATOM   1764  CA  TRP A 240       9.420  28.913  -9.382  1.00 21.13      A    C
ATOM   1765  CB  TRP A 240      10.192  28.842  -8.055  1.00 21.05      A    C
ATOM   1766  CG  TRP A 240       9.324  28.850  -6.857  1.00 22.76      A    C
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ATOM   1767  CD1 TRP A 240       8.027  28.446  -6.782  1.00 23.97      A    C
ATOM   1768  NE1 TRP A 240       7.548  28.624  -5.509  1.00 24.62      A    N
ATOM   1769  CE2 TRP A 240       8.547  29.148  -4.726  1.00 24.31      A    C
ATOM   1770  CD2 TRP A 240       9.677  29.302  -5.537  1.00 23.24      A    C
ATOM   1771  CE3 TRP A 240      10.839  29.811  -4.966  1.00 24.95      A    C
ATOM   1772  CZ3 TRP A 240      10.833  30.146  -3.637  1.00 24.14      A    C
ATOM   1773  CH2 TRP A 240       9.682  29.991  -2.857  1.00 23.89      A    C
ATOM   1774  CZ2 TRP A 240       8.542  29.483  -3.378  1.00 25.05      A    C
ATOM   1775  C   TRP A 240      10.355  29.466 -10.461  1.00 20.95      A    C
ATOM   1776  O   TRP A 240      10.419  30.673 -10.703  1.00 20.42      A    O
ATOM   1777  N   ALA A 241      11.097  28.566 -11.080  1.00 21.11      A    N
ATOM   1778  CA  ALA A 241      12.022  28.907 -12.149  1.00 21.52      A    C
ATOM   1779  CB  ALA A 241      13.243  29.629 -11.606  1.00 21.93      A    C
ATOM   1780  C   ALA A 241      12.466  27.641 -12.801  1.00 21.79      A    C
ATOM   1781  O   ALA A 241      12.440  26.569 -12.169  1.00 22.05      A    O
ATOM   1782  N   ASN A 242      12.929  27.769 -14.040  1.00 22.09      A    N
ATOM   1783  CA  ASN A 242      13.481  26.656 -14.800  1.00 22.74      A    C
ATOM   1784  CB  ASN A 242      13.397  26.962 -16.322  1.00 22.69      A    C
ATOM   1785  CG  ASN A 242      11.960  27.071 -16.828  1.00 22.96      A    C
ATOM   1786  OD1 ASN A 242      11.024  26.578 -16.198  1.00 21.33      A    O
ATOM   1787  ND2 ASN A 242      11.782  27.727 -17.969  1.00 21.31      A    N
ATOM   1788  C   ASN A 242      14.927  26.359 -14.458  1.00 23.18      A    C
ATOM   1789  O   ASN A 242      15.634  27.194 -13.902  1.00 23.35      A    O
ATOM   1790  N   HIS A 243      15.375  25.169 -14.820  1.00 24.21      A    N
ATOM   1791  CA  HIS A 243      16.802  24.875 -14.862  1.00 25.06      A    C
ATOM   1792  CB  HIS A 243      17.234  24.062 -13.653  1.00 25.31      A    C
ATOM   1793  CG  HIS A 243      18.703  23.809 -13.595  1.00 27.16      A    C
ATOM   1794  ND1 HIS A 243      19.599  24.733 -13.086  1.00 30.11      A    N
ATOM   1795  CE1 HIS A 243      20.820  24.231 -13.152  1.00 30.29      A    C
ATOM   1796  NE2 HIS A 243      20.752  23.036 -13.713  1.00 29.63      A    N
ATOM   1797  CD2 HIS A 243      19.442  22.754 -14.008  1.00 28.73      A    C
ATOM   1798  C   HIS A 243      17.158  24.144 -16.162  1.00 26.02      A    C
ATOM   1799  O   HIS A 243      17.851  24.726 -17.003  1.00 25.77      A    O
ATOM   1800  N   ASP A 244      16.711  22.880 -16.299  1.00 26.20      A    N
ATOM   1801  CA  ASP A 244      16.757  22.137 -17.584  1.00 27.35      A    C
ATOM   1802  CB  ASP A 244      17.972  21.252 -17.646  1.00 28.02      A    C
ATOM   1803  CG  ASP A 244      18.211  20.272 -16.546  1.00 29.28      A    C
ATOM   1804  OD1 ASP A 244      19.393  20.188 -16.099  1.00 34.73      A    O
ATOM   1805  OD2 ASP A 244      17.310  19.568 -16.056  1.00 28.43      A    O
ATOM   1806  C   ASP A 244      15.427  21.429 -17.760  1.00 27.57      A    C
ATOM   1807  O   ASP A 244      14.751  21.208 -16.721  1.00 27.11      A    O
ATOM   1808  N   SER A 245      15.290  20.734 -18.836  1.00 27.83      A    N
ATOM   1809  CA  SER A 245      14.559  19.557 -19.209  1.00 26.73      A    C
ATOM   1810  CB  SER A 245      15.083  18.972 -20.483  1.00 26.99      A    C
ATOM   1811  OG  SER A 245      15.792  17.785 -20.481  1.00 27.12      A    O
ATOM   1812  C   SER A 245      14.234  18.594 -18.102  1.00 25.28      A    C
ATOM   1813  O   SER A 245      13.146  17.973 -18.152  1.00 24.66      A    O
ATOM   1814  N   LYS A 246      15.122  18.339 -17.176  1.00 23.51      A    N
ATOM   1815  CA  LYS A 246      14.918  17.304 -16.177  1.00 22.90      A    C
ATOM   1816  CB  LYS A 246      15.977  16.205 -16.332  1.00 23.64      A    C
ATOM   1817  CG  LYS A 246      15.852  15.384 -17.600  1.00 26.42      A    C
ATOM   1818  CD  LYS A 246      17.094  14.548 -17.859  1.00 29.39      A    C
ATOM   1819  CE  LYS A 246      16.880  13.584 -19.018  1.00 32.94      A    C
ATOM   1820  NZ  LYS A 246      18.070  13.501 -19.908  1.00 37.30      A    N
ATOM   1821  C   LYS A 246      14.812  17.762 -14.740  1.00 21.77      A    C
ATOM   1822  O   LYS A 246      14.396  17.059 -13.828  1.00 19.24      A    O
ATOM   1823  N   TYR A 247      15.126  19.026 -14.452  1.00 20.43      A    N
ATOM   1824  CA  TYR A 247      15.144  19.544 -13.079  1.00 19.83      A    C
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ATOM   1825  CB  TYR A 247      16.541  19.398 -12.456  1.00 19.35      A    C
ATOM   1826  CG  TYR A 247      17.007  17.966 -12.434  1.00 19.14      A    C
ATOM   1827  CD1 TYR A 247      17.784  17.442 -13.482  1.00 21.08      A    C
ATOM   1828  CE1 TYR A 247      18.170  16.121 -13.489  1.00 17.97      A    C
ATOM   1829  CZ  TYR A 247      17.780  15.292 -12.458  1.00 19.97      A    C
ATOM   1830  OH  TYR A 247      18.159  13.964 -12.465  1.00 18.06      A    O
ATOM   1831  CE2 TYR A 247      16.999  15.781 -11.417  1.00 18.19      A    C
ATOM   1832  CD2 TYR A 247      16.630  17.109 -11.408  1.00 19.09      A    C
ATOM   1833  C   TYR A 247      14.697  21.003 -13.069  1.00 18.89      A    C
ATOM   1834  O   TYR A 247      15.017  21.761 -13.994  1.00 18.71      A    O
ATOM   1835  N   ALA A 248      13.936  21.385 -12.046  1.00 17.07      A    N
ATOM   1836  CA  ALA A 248      13.512  22.769 -11.893  1.00 16.28      A    C
ATOM   1837  CB  ALA A 248      12.294  23.035 -12.733  1.00 15.85      A    C
ATOM   1838  C   ALA A 248      13.253  23.110 -10.425  1.00 15.75      A    C
ATOM   1839  O   ALA A 248      13.358  22.236  -9.549  1.00 15.81      A    O
ATOM   1840  N   TYR A 249      12.956  24.384 -10.174  1.00 15.33      A    N
ATOM   1841  CA  TYR A 249      12.910  24.949  -8.832  1.00 15.08      A    C
ATOM   1842  CB  TYR A 249      13.520  26.336  -8.802  1.00 15.54      A    C
ATOM   1843  CG  TYR A 249      14.999  26.398  -9.087  1.00 15.33      A    C
ATOM   1844  CD1 TYR A 249      15.470  26.675 -10.370  1.00 17.29      A    C
ATOM   1845  CE1 TYR A 249      16.829  26.754 -10.640  1.00 16.19      A    C
ATOM   1846  CZ  TYR A 249      17.741  26.557  -9.608  1.00 18.72      A    C
ATOM   1847  OH  TYR A 249      19.088  26.649  -9.839  1.00 21.92      A    O
ATOM   1848  CE2 TYR A 249      17.306  26.287  -8.330  1.00 18.20      A    C
ATOM   1849  CD2 TYR A 249      15.930  26.207  -8.070  1.00 17.03      A    C
ATOM   1850  C   TYR A 249      11.497  25.078  -8.358  1.00 15.50      A    C
ATOM   1851  O   TYR A 249      10.599  25.480  -9.122  1.00 16.06      A    O
ATOM   1852  N   MET A 250      11.291  24.749  -7.082  1.00 15.10      A    N
ATOM   1853  CA  MET A 250      10.015  24.967  -6.430  1.00 15.40      A    C
ATOM   1854  CB  MET A 250       9.153  23.703  -6.542  1.00 15.90      A    C
ATOM   1855  CG  MET A 250       7.677  23.947  -6.729  1.00 19.64      A    C
ATOM   1856  SD  MET A 250       6.677  22.370  -6.869  1.00 23.44      A    S
ATOM   1857  CE  MET A 250       7.321  21.709  -8.163  1.00 22.96      A    C
ATOM   1858  C   MET A 250      10.274  25.318  -4.966  1.00 15.09      A    C
ATOM   1859  O   MET A 250      11.366  25.081  -4.440  1.00 15.78      A    O
ATOM   1860  N   GLY A 251       9.279  25.888  -4.314  1.00 14.69      A    N
ATOM   1861  CA  GLY A 251       9.373  26.203  -2.902  1.00 13.76      A    C
ATOM   1862  C   GLY A 251       8.026  26.058  -2.248  1.00 14.49      A    C
ATOM   1863  O   GLY A 251       6.984  26.057  -2.933  1.00 13.60      A    O
ATOM   1864  N   GLY A 252       8.056  25.926  -0.920  1.00 12.84      A    N
ATOM   1865  CA  GLY A 252       6.879  25.694  -0.101  1.00 13.22      A    C
ATOM   1866  C   GLY A 252       7.242  24.765   1.058  1.00 12.42      A    C
ATOM   1867  O   GLY A 252       8.354  24.185   1.073  1.00 11.46      A    O
ATOM   1868  N   THR A 253       6.328  24.598   2.008  1.00 12.37      A    N
ATOM   1869  CA  THR A 253       6.518  23.583   3.043  1.00 12.51      A    C
ATOM   1870  CB  THR A 253       5.543  23.697   4.256  1.00 13.05      A    C
ATOM   1871  OG1 THR A 253       4.138  23.788   3.858  1.00 11.78      A    O
ATOM   1872  CG2 THR A 253       5.837  24.964   5.042  1.00 13.23      A    C
ATOM   1873  C   THR A 253       6.463  22.211   2.396  1.00 12.60      A    C
ATOM   1874  O   THR A 253       6.945  21.239   2.966  1.00 12.54      A    O
ATOM   1875  N   SER A 254       5.902  22.158   1.187  1.00 12.69      A    N
ATOM   1876  CA  SER A 254       5.905  20.957   0.357  1.00 12.54      A    C
ATOM   1877  CB  SER A 254       5.228  21.233  -0.994  1.00 12.41      A    C
ATOM   1878  OG  SER A 254       3.822  21.002  -0.960  1.00 11.90      A    O
ATOM   1879  C   SER A 254       7.298  20.445   0.050  1.00 12.52      A    C
ATOM   1880  O   SER A 254       7.459  19.253  -0.150  1.00 12.45      A    O
ATOM   1881  N   MET A 255       8.255  21.361  -0.054  1.00 12.52      A    N
ATOM   1882  CA  MET A 255       9.640  21.062  -0.385  1.00 13.23      A    C
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ATOM   1883  CB  MET A 255      10.260  22.231  -1.164  1.00 13.16      A    C
ATOM   1884  CG  MET A 255       9.955  22.255  -2.667  1.00 13.61      A    C
ATOM   1885  SD  MET A 255       8.220  22.693  -3.027  1.00 16.25      A    S
ATOM   1886  CE  MET A 255       7.683  21.071  -3.591  1.00 13.35      A    C
ATOM   1887  C   MET A 255      10.478  20.759   0.873  1.00 13.32      A    C
ATOM   1888  O   MET A 255      11.396  19.934   0.847  1.00 13.21      A    O
ATOM   1889  N   ALA A 256      10.162  21.415   1.981  1.00 12.98      A    N
ATOM   1890  CA  ALA A 256      10.904  21.161   3.213  1.00 12.47      A    C
ATOM   1891  CB  ALA A 256      10.516  22.175   4.265  1.00 11.99      A    C
ATOM   1892  C   ALA A 256      10.645  19.737   3.717  1.00 11.89      A    C
ATOM   1893  O   ALA A 256      11.553  19.018   4.179  1.00 11.48      A    O
ATOM   1894  N   THR A 257       9.390  19.341   3.629  1.00 11.55      A    N
ATOM   1895  CA  THR A 257       8.944  18.065   4.146  1.00 11.50      A    C
ATOM   1896  CB  THR A 257       7.423  17.938   3.908  1.00 12.07      A    C
ATOM   1897  OG1 THR A 257       6.754  19.013   4.569  1.00 13.08      A    O
ATOM   1898  CG2 THR A 257       6.838  16.661   4.540  1.00 12.46      A    C
ATOM   1899  C   THR A 257       9.705  16.849   3.587  1.00 11.20      A    C
ATOM   1900  O   THR A 257      10.172  16.018   4.382  1.00 11.03      A    O
ATOM   1901  N   PRO A 258       9.781  16.686   2.259  1.00 11.22      A    N
ATOM   1902  CA  PRO A 258      10.466  15.521   1.687  1.00 10.92      A    C
ATOM   1903  CB  PRO A 258      10.200  15.644   0.182  1.00 10.45      A    C
ATOM   1904  CG  PRO A 258       9.884  17.057  -0.029  1.00 11.62      A    C
ATOM   1905  CD  PRO A 258       9.164  17.504   1.207  1.00 10.92      A    C
ATOM   1906  C   PRO A 258      11.969  15.503   1.976  1.00 10.83      A    C
ATOM   1907  O   PRO A 258      12.524  14.417   2.020  1.00  9.95      A    O
ATOM   1908  N   ILE A 259      12.605  16.665   2.160  1.00 11.19      A    N
ATOM   1909  CA  ILE A 259      14.004  16.711   2.597  1.00 11.51      A    C
ATOM   1910  CB  ILE A 259      14.439  18.183   2.712  1.00 11.81      A    C
ATOM   1911  CG1 ILE A 259      14.492  18.843   1.314  1.00 14.15      A    C
ATOM   1912  CD1 ILE A 259      15.690  18.403   0.504  1.00 17.31      A    C
ATOM   1913  CG2 ILE A 259      15.790  18.313   3.375  1.00 11.02      A    C
ATOM   1914  C   ILE A 259      14.147  15.975   3.950  1.00 11.56      A    C
ATOM   1915  O   ILE A 259      15.038  15.133   4.124  1.00 11.81      A    O
ATOM   1916  N   VAL A 260      13.259  16.295   4.886  1.00 11.02      A    N
ATOM   1917  CA  VAL A 260      13.244  15.668   6.199  1.00 12.26      A    C
ATOM   1918  CB  VAL A 260      12.301  16.412   7.150  1.00 12.30      A    C
ATOM   1919  CG1 VAL A 260      12.286  15.743   8.557  1.00 12.78      A    C
ATOM   1920  CG2 VAL A 260      12.721  17.855   7.268  1.00 13.51      A    C
ATOM   1921  C   VAL A 260      12.847  14.185   6.106  1.00 12.24      A    C
ATOM   1922  O   VAL A 260      13.412  13.339   6.786  1.00 12.79      A    O
ATOM   1923  N   ALA A 261      11.922  13.864   5.217  1.00 12.41      A    N
ATOM   1924  CA  ALA A 261      11.530  12.480   4.997  1.00 11.93      A    C
ATOM   1925  CB  ALA A 261      10.426  12.376   3.920  1.00 12.16      A    C
ATOM   1926  C   ALA A 261      12.750  11.661   4.585  1.00 11.91      A    C
ATOM   1927  O   ALA A 261      12.943  10.560   5.055  1.00 11.34      A    O
ATOM   1928  N   GLY A 262      13.550  12.186   3.665  1.00 12.22      A    N
ATOM   1929  CA  GLY A 262      14.794  11.533   3.291  1.00 12.29      A    C
ATOM   1930  C   GLY A 262      15.786  11.431   4.447  1.00 12.34      A    C
ATOM   1931  O   GLY A 262      16.414  10.386   4.660  1.00 11.90      A    O
ATOM   1932  N   ASN A 263      15.901  12.490   5.243  1.00 12.20      A    N
ATOM   1933  CA  ASN A 263      16.744  12.433   6.435  1.00 11.84      A    C
ATOM   1934  CB  ASN A 263      16.772  13.773   7.170  1.00 12.31      A    C
ATOM   1935  CG  ASN A 263      17.389  14.887   6.351  1.00 13.12      A    C
ATOM   1936  OD1 ASN A 263      18.326  14.681   5.525  1.00 15.95      A    O
ATOM   1937  ND2 ASN A 263      16.924  16.073   6.600  1.00  9.15      A    N
ATOM   1938  C   ASN A 263      16.289  11.348   7.396  1.00 11.83      A    C
ATOM   1939  O   ASN A 263      17.112  10.672   8.020  1.00 11.88      A    O
ATOM   1940  N   VAL A 264      14.983  11.181   7.517  1.00 11.77      A    N
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ATOM   1941  CA  VAL A 264      14.425  10.138   8.367  1.00 12.33      A    C
ATOM   1942  CB  VAL A 264      12.893  10.268   8.506  1.00 12.44      A    C
ATOM   1943  CG1 VAL A 264      12.280   9.045   9.178  1.00 12.44      A    C
ATOM   1944  CG2 VAL A 264      12.543  11.471   9.323  1.00 13.22      A    C
ATOM   1945  C   VAL A 264      14.817   8.754   7.843  1.00 11.95      A    C
ATOM   1946  O   VAL A 264      15.164   7.896   8.625  1.00 12.24      A    O
ATOM   1947  N   ALA A 265      14.813   8.553   6.527  1.00 12.03      A    N
ATOM   1948  CA  ALA A 265      15.279   7.292   5.966  1.00 11.47      A    C
ATOM   1949  CB  ALA A 265      15.018   7.237   4.460  1.00 11.96      A    C
ATOM   1950  C   ALA A 265      16.746   7.046   6.293  1.00 11.77      A    C
ATOM   1951  O   ALA A 265      17.139   5.932   6.592  1.00 11.77      A    O
ATOM   1952  N   GLN A 266      17.571   8.091   6.262  1.00 12.48      A    N
ATOM   1953  CA  GLN A 266      18.999   7.940   6.586  1.00 11.99      A    C
ATOM   1954  CB  GLN A 266      19.782   9.230   6.311  1.00 10.90      A    C
ATOM   1955  CG  GLN A 266      19.786   9.691   4.865  1.00 12.48      A    C
ATOM   1956  CD  GLN A 266      20.548  11.011   4.671  1.00 12.24      A    C
ATOM   1957  OE1 GLN A 266      21.762  11.028   4.352  1.00 16.02      A    O
ATOM   1958  NE2 GLN A 266      19.857  12.088   4.853  1.00  8.53      A    N
ATOM   1959  C   GLN A 266      19.159   7.571   8.046  1.00 12.14      A    C
ATOM   1960  O   GLN A 266      19.927   6.688   8.398  1.00 12.13      A    O
ATOM   1961  N   LEU A 267      18.463   8.305   8.898  1.00 12.44      A    N
ATOM   1962  CA  LEU A 267      18.473   8.049  10.317  1.00 12.06      A    C
ATOM   1963  CB  LEU A 267      17.624   9.107  11.014  1.00 12.45      A    C
ATOM   1964  CG  LEU A 267      17.550   9.097  12.540  1.00 12.15      A    C
ATOM   1965  CD1 LEU A 267      18.918   9.293  13.116  1.00 12.99      A    C
ATOM   1966  CD2 LEU A 267      16.616  10.187  13.009  1.00 12.84      A    C
ATOM   1967  C   LEU A 267      17.984   6.649  10.654  1.00 12.72      A    C
ATOM   1968  O   LEU A 267      18.581   5.972  11.497  1.00 12.91      A    O
ATOM   1969  N   ARG A 268      16.872   6.219  10.044  1.00 12.54      A    N
ATOM   1970  CA  ARG A 268      16.295   4.886  10.321  1.00 12.31      A    C
ATOM   1971  CB  ARG A 268      14.961   4.722   9.577  1.00 12.21      A    C
ATOM   1972  CG  ARG A 268      14.016   3.635  10.155  1.00 12.56      A    C
ATOM   1973  CD  ARG A 268      12.652   3.605   9.510  1.00 14.20      A    C
ATOM   1974  NE  ARG A 268      11.781   2.591  10.105  1.00 14.70      A    N
ATOM   1975  CZ  ARG A 268      11.837   1.306   9.829  1.00 14.81      A    C
ATOM   1976  NH1 ARG A 268      12.697   0.829   8.942  1.00 14.11      A    N
ATOM   1977  NH2 ARG A 268      10.993   0.483  10.432  1.00 15.99      A    N
ATOM   1978  C   ARG A 268      17.284   3.763   9.929  1.00 12.37      A    C
ATOM   1979  O   ARG A 268      17.533   2.837  10.689  1.00 11.86      A    O
ATOM   1980  N   GLU A 269      17.846   3.870   8.729  1.00 11.97      A    N
ATOM   1981  CA  GLU A 269      18.965   3.026   8.306  1.00 12.12      A    C
ATOM   1982  CB  GLU A 269      19.561   3.537   6.993  1.00 11.36      A    C
ATOM   1983  CG  GLU A 269      20.764   2.715   6.542  1.00 12.78      A    C
ATOM   1984  CD  GLU A 269      21.477   3.260   5.335  1.00 15.24      A    C
ATOM   1985  OE1 GLU A 269      21.277   4.447   5.007  1.00 16.05      A    O
ATOM   1986  OE2 GLU A 269      22.246   2.479   4.711  1.00 16.25      A    O
ATOM   1987  C   GLU A 269      20.082   2.954   9.354  1.00 12.56      A    C
ATOM   1988  O   GLU A 269      20.596   1.875   9.645  1.00 12.26      A    O
ATOM   1989  N   HIS A 270      20.482   4.104   9.894  1.00 12.79      A    N
ATOM   1990  CA  HIS A 270      21.556   4.119  10.859  1.00 12.79      A    C
ATOM   1991  CB  HIS A 270      21.918   5.531  11.289  1.00 12.76      A    C
ATOM   1992  CG BHIS A 270      23.160   5.583  12.120  0.50 10.01      A    C
ATOM   1993  CG AHIS A 270      23.195   5.601  12.063  0.50 15.58      A    C
ATOM   1994  ND1BHIS A 270      23.186   6.137  13.385  0.50  7.23      A    N
ATOM   1995  ND1AHIS A 270      23.243   5.459  13.432  0.50 20.08      A    N
ATOM   1996  CE1BHIS A 270      24.404   6.019  13.885  0.50  6.26      A    C
ATOM   1997  CE1AHIS A 270      24.498   5.548  13.839  0.50 20.34      A    C
ATOM   1998  NE2BHIS A 270      25.163   5.387  13.000  0.50  8.61      A    N
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ATOM   1999  NE2AHIS A 270      25.265   5.744  12.783  0.50 20.61      A    N
ATOM   2000  CD2BHIS A 270      24.405   5.102  11.888  0.50  6.18      A    C
ATOM   2001  CD2AHIS A 270      24.475   5.782  11.659  0.50 18.53      A    C
ATOM   2002  C    HIS A 270      21.210   3.294  12.099  1.00 12.75      A    C
ATOM   2003  O    HIS A 270      22.031   2.541  12.562  1.00 12.88      A    O
ATOM   2004  N    PHE A 271      20.009   3.468  12.666  1.00 12.25      A    N
ATOM   2005  CA   PHE A 271      19.642   2.680  13.834  1.00 12.36      A    C
ATOM   2006  CB   PHE A 271      18.274   3.114  14.370  1.00 12.01      A    C
ATOM   2007  CG   PHE A 271      18.328   4.292  15.293  1.00 11.54      A    C
ATOM   2008  CD1  PHE A 271      18.557   4.127  16.643  1.00 12.44      A    C
ATOM   2009  CE1  PHE A 271      18.601   5.229  17.500  1.00 13.55      A    C
ATOM   2010  CZ   PHE A 271      18.400   6.479  17.016  1.00 11.92      A    C
ATOM   2011  CE2  PHE A 271      18.145   6.655  15.663  1.00 15.14      A    C
ATOM   2012  CD2  PHE A 271      18.096   5.567  14.820  1.00 13.90      A    C
ATOM   2013  C    PHE A 271      19.620   1.178  13.492  1.00 13.05      A    C
ATOM   2014  O    PHE A 271      20.147   0.341  14.240  1.00 15.06      A    O
ATOM   2015  N    VAL A 272      19.007   0.850  12.371  1.00 12.88      A    N
ATOM   2016  CA   VAL A 272      18.765  -0.526  11.961  1.00 13.79      A    C
ATOM   2017  CB   VAL A 272      17.856  -0.539  10.706  1.00 13.45      A    C
ATOM   2018  CG1  VAL A 272      17.977  -1.840   9.953  1.00 15.25      A    C
ATOM   2019  CG2  VAL A 272      16.429  -0.264  11.112  1.00 13.55      A    C
ATOM   2020  C    VAL A 272      20.068  -1.276  11.689  1.00 14.17      A    C
ATOM   2021  O    VAL A 272      20.242  -2.415  12.162  1.00 14.67      A    O
ATOM   2022  N    LYS A 273      20.992  -0.619  10.990  1.00 14.25      A    N
ATOM   2023  CA   LYS A 273      22.255  -1.217  10.606  1.00 14.60      A    C
ATOM   2024  CB   LYS A 273      22.759  -0.664   9.267  1.00 14.93      A    C
ATOM   2025  CG   LYS A 273      21.893  -1.085   8.052  1.00 15.97      A    C
ATOM   2026  CD   LYS A 273      22.432  -0.488   6.729  1.00 14.97      A    C
ATOM   2027  CE   LYS A 273      21.735  -1.010   5.482  1.00 16.43      A    C
ATOM   2028  NZ   LYS A 273      22.131  -0.162   4.300  1.00 13.02      A    N
ATOM   2029  C    LYS A 273      23.366  -1.133  11.645  1.00 14.97      A    C
ATOM   2030  O    LYS A 273      24.172  -2.075  11.740  1.00 12.32      A    O
ATOM   2031  N    ASN A 274      23.402  -0.033  12.403  1.00 14.72      A    N
ATOM   2032  CA   ASN A 274      24.556   0.298  13.225  1.00 15.62      A    C
ATOM   2033  CB   ASN A 274      25.197   1.649  12.786  1.00 16.07      A    C
ATOM   2034  CG   ASN A 274      25.555   1.662  11.290  1.00 17.59      A    C
ATOM   2035  OD1  ASN A 274      25.285   2.647  10.543  1.00 18.70      A    O
ATOM   2036  ND2  ASN A 274      26.124   0.561  10.839  1.00 13.05      A    N
ATOM   2037  C    ASN A 274      24.253   0.365  14.694  1.00 15.60      A    C
ATOM   2038  O    ASN A 274      25.165   0.449  15.465  1.00 15.70      A    O
ATOM   2039  N    ARG A 275      22.979   0.348  15.092  1.00 14.80      A    N
ATOM   2040  CA   ARG A 275      22.670   0.517  16.505  1.00 15.19      A    C
ATOM   2041  CB   ARG A 275      22.046   1.883  16.723  1.00 14.89      A    C
ATOM   2042  CG   ARG A 275      22.925   3.001  16.141  1.00 17.88      A    C
ATOM   2043  CD   ARG A 275      22.682   4.354  16.748  1.00 17.97      A    C
ATOM   2044  NE   ARG A 275      23.098   4.391  18.146  1.00 15.44      A    N
ATOM   2045  CZ   ARG A 275      22.783   5.383  18.977  1.00 18.17      A    C
ATOM   2046  NH1  ARG A 275      22.080   6.422  18.540  1.00 17.27      A    N
ATOM   2047  NH2  ARG A 275      23.191   5.356  20.239  1.00 17.72      A    N
ATOM   2048  C    ARG A 275      21.796  -0.573  17.088  1.00 14.64      A    C
ATOM   2049  O    ARG A 275      21.382  -0.456  18.212  1.00 15.75      A    O
ATOM   2050  N    GLY A 276      21.459  -1.577  16.283  1.00 14.66      A    N
ATOM   2051  CA   GLY A 276      20.880  -2.825  16.771  1.00 14.63      A    C
ATOM   2052  C    GLY A 276      19.403  -2.811  17.060  1.00 14.40      A    C
ATOM   2053  O    GLY A 276      18.863  -3.751  17.664  1.00 13.52      A    O
ATOM   2054  N    VAL A 277      18.729  -1.745  16.638  1.00 14.10      A    N
ATOM   2055  CA   VAL A 277      17.318  -1.618  16.894  1.00 14.10      A    C
ATOM   2056  CB   VAL A 277      17.021  -0.657  18.097  1.00 14.71      A    C
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ATOM   2057  CG1 VAL A 277      17.768  -1.058  19.354  1.00 14.49      A    C
ATOM   2058  CG2 VAL A 277      17.268   0.771  17.733  1.00 15.67      A    C
ATOM   2059  C   VAL A 277      16.547  -1.097  15.689  1.00 13.79      A    C
ATOM   2060  O   VAL A 277      17.082  -0.372  14.853  1.00 14.29      A    O
ATOM   2061  N   THR A 278      15.273  -1.472  15.607  1.00 14.21      A    N
ATOM   2062  CA  THR A 278      14.325  -0.778  14.749  1.00 14.50      A    C
ATOM   2063  CB  THR A 278      13.187  -1.700  14.301  1.00 15.23      A    C
ATOM   2064  OG1 THR A 278      13.744  -2.825  13.607  1.00 19.10      A    O
ATOM   2065  CG2 THR A 278      12.304  -0.986  13.245  1.00 17.53      A    C
ATOM   2066  C   THR A 278      13.760   0.394  15.526  1.00 13.49      A    C
ATOM   2067  O   THR A 278      13.028   0.210  16.485  1.00 13.51      A    O
ATOM   2068  N   PRO A 279      14.104   1.612  15.134  1.00 12.55      A    N
ATOM   2069  CA  PRO A 279      13.679   2.803  15.896  1.00 11.32      A    C
ATOM   2070  CB  PRO A 279      14.520   3.920  15.277  1.00 11.71      A    C
ATOM   2071  CG  PRO A 279      14.682   3.493  13.842  1.00 11.40      A    C
ATOM   2072  CD  PRO A 279      14.817   1.975  13.895  1.00 12.28      A    C
ATOM   2073  C   PRO A 279      12.211   3.055  15.672  1.00 11.90      A    C
ATOM   2074  O   PRO A 279      11.786   3.053  14.516  1.00 12.19      A    O
ATOM   2075  N   LYS A 280      11.438   3.212  16.743  1.00 11.50      A    N
ATOM   2076  CA  LYS A 280      10.020   3.518  16.639  1.00 12.77      A    C
ATOM   2077  CB  LYS A 280       9.354   3.389  18.024  1.00 13.46      A    C
ATOM   2078  CG  LYS A 280       9.324   1.993  18.573  1.00 15.21      A    C
ATOM   2079  CD  LYS A 280       8.273   1.192  17.861  1.00 20.42      A    C
ATOM   2080  CE  LYS A 280       8.012  -0.146  18.555  1.00 23.45      A    C
ATOM   2081  NZ  LYS A 280       6.935  -0.858  17.808  1.00 26.12      A    N
ATOM   2082  C   LYS A 280       9.811   4.951  16.120  1.00 11.96      A    C
ATOM   2083  O   LYS A 280      10.710   5.782  16.200  1.00 13.23      A    O
ATOM   2084  N   PRO A 281       8.666   5.233  15.512  1.00 12.23      A    N
ATOM   2085  CA  PRO A 281       8.370   6.608  15.073  1.00 11.69      A    C
ATOM   2086  CB  PRO A 281       6.897   6.540  14.763  1.00 12.25      A    C
ATOM   2087  CG  PRO A 281       6.755   5.162  14.210  1.00 12.66      A    C
ATOM   2088  CD  PRO A 281       7.592   4.300  15.126  1.00 11.87      A    C
ATOM   2089  C   PRO A 281       8.682   7.678  16.105  1.00 11.94      A    C
ATOM   2090  O   PRO A 281       9.287   8.708  15.734  1.00 11.60      A    O
ATOM   2091  N   SER A 282       8.303   7.447  17.374  1.00 11.91      A    N
ATOM   2092  CA  SER A 282       8.579   8.404  18.442  1.00 11.78      A    C
ATOM   2093  CB  SER A 282       8.017   7.930  19.789  1.00 11.85      A    C
ATOM   2094  OG  SER A 282       8.503   6.639  20.117  1.00 12.30      A    O
ATOM   2095  C   SER A 282      10.049   8.704  18.654  1.00 11.36      A    C
ATOM   2096  O   SER A 282      10.402   9.835  19.014  1.00 11.10      A    O
ATOM   2097  N   LEU A 283      10.896   7.696  18.498  1.00 11.81      A    N
ATOM   2098  CA  LEU A 283      12.332   7.889  18.642  1.00 11.66      A    C
ATOM   2099  CB  LEU A 283      13.042   6.532  18.856  1.00 11.73      A    C
ATOM   2100  CG  LEU A 283      14.575   6.628  18.893  1.00 11.60      A    C
ATOM   2101  CD1 LEU A 283      15.029   7.501  20.001  1.00 10.08      A    C
ATOM   2102  CD2 LEU A 283      15.180   5.233  19.066  1.00 15.86      A    C
ATOM   2103  C   LEU A 283      12.953   8.650  17.465  1.00 11.15      A    C
ATOM   2104  O   LEU A 283      13.812   9.515  17.644  1.00 11.72      A    O
ATOM   2105  N   LEU A 284      12.575   8.305  16.244  1.00 11.65      A    N
ATOM   2106  CA  LEU A 284      13.056   9.058  15.088  1.00 10.89      A    C
ATOM   2107  CB  LEU A 284      12.493   8.470  13.802  1.00 10.71      A    C
ATOM   2108  CG  LEU A 284      13.010   7.059  13.442  1.00 10.82      A    C
ATOM   2109  CD1 LEU A 284      12.102   6.419  12.399  1.00 10.74      A    C
ATOM   2110  CD2 LEU A 284      14.425   7.107  12.953  1.00 10.79      A    C
ATOM   2111  C   LEU A 284      12.741  10.568  15.245  1.00 10.24      A    C
ATOM   2112  O   LEU A 284      13.591  11.414  15.013  1.00  9.64      A    O
ATOM   2113  N   LYS A 285      11.527  10.868  15.682  1.00 10.77      A    N
ATOM   2114  CA  LYS A 285      11.054  12.217  15.890  1.00 10.81      A    C
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ATOM   2115  CB  LYS A 285       9.544  12.188  16.152  1.00 10.59      A    C
ATOM   2116  CG  LYS A 285       8.909  13.531  16.527  1.00 10.18      A    C
ATOM   2117  CD  LYS A 285       7.372  13.380  16.583  1.00 12.54      A    C
ATOM   2118  CE  LYS A 285       6.660  14.630  17.085  1.00 11.16      A    C
ATOM   2119  NZ  LYS A 285       5.159  14.525  16.941  1.00  9.27      A    N
ATOM   2120  C   LYS A 285      11.816  12.886  17.037  1.00 10.86      A    C
ATOM   2121  O   LYS A 285      12.287  13.995  16.888  1.00 11.16      A    O
ATOM   2122  N   ALA A 286      11.964  12.194  18.156  1.00 10.94      A    N
ATOM   2123  CA  ALA A 286      12.744  12.722  19.280  1.00 11.16      A    C
ATOM   2124  CB  ALA A 286      12.657  11.813  20.437  1.00 11.37      A    C
ATOM   2125  C   ALA A 286      14.206  12.952  18.897  1.00 10.98      A    C
ATOM   2126  O   ALA A 286      14.794  13.947  19.275  1.00 10.07      A    O
ATOM   2127  N   ALA A 287      14.778  12.048  18.115  1.00 11.61      A    N
ATOM   2128  CA  ALA A 287      16.175  12.206  17.679  1.00 12.13      A    C
ATOM   2129  CB  ALA A 287      16.692  10.922  17.034  1.00 11.58      A    C
ATOM   2130  C   ALA A 287      16.349  13.411  16.742  1.00 12.42      A    C
ATOM   2131  O   ALA A 287      17.310  14.165  16.873  1.00 11.82      A    O
ATOM   2132  N   LEU A 288      15.407  13.623  15.826  1.00 12.37      A    N
ATOM   2133  CA  LEU A 288      15.473  14.808  14.956  1.00 13.09      A    C
ATOM   2134  CB  LEU A 288      14.357  14.775  13.917  1.00 13.67      A    C
ATOM   2135  CG  LEU A 288      14.552  13.833  12.736  1.00 15.39      A    C
ATOM   2136  CD1 LEU A 288      13.379  14.033  11.840  1.00 19.44      A    C
ATOM   2137  CD2 LEU A 288      15.842  14.113  11.974  1.00 15.17      A    C
ATOM   2138  C   LEU A 288      15.329  16.105  15.747  1.00 12.69      A    C
ATOM   2139  O   LEU A 288      16.014  17.107  15.481  1.00 12.69      A    O
ATOM   2140  N   ILE A 289      14.412  16.096  16.704  1.00 12.33      A    N
ATOM   2141  CA  ILE A 289      14.195  17.261  17.546  1.00 12.69      A    C
ATOM   2142  CB  ILE A 289      12.920  17.084  18.397  1.00 12.55      A    C
ATOM   2143  CG1 ILE A 289      11.688  17.178  17.488  1.00 11.46      A    C
ATOM   2144  CD1 ILE A 289      10.404  16.725  18.104  1.00 10.00      A    C
ATOM   2145  CG2 ILE A 289      12.869  18.098  19.506  1.00 13.54      A    C
ATOM   2146  C   ILE A 289      15.412  17.596  18.426  1.00 12.74      A    C
ATOM   2147  O   ILE A 289      15.844  18.746  18.442  1.00 13.36      A    O
ATOM   2148  N   ALA A 290      15.975  16.612  19.132  1.00 11.71      A    N
ATOM   2149  CA  ALA A 290      17.132  16.854  19.976  1.00 11.73      A    C
ATOM   2150  CB  ALA A 290      17.529  15.593  20.698  1.00 12.08      A    C
ATOM   2151  C   ALA A 290      18.326  17.370  19.191  1.00 11.95      A    C
ATOM   2152  O   ALA A 290      19.114  18.198  19.689  1.00 10.65      A    O
ATOM   2153  N   GLY A 291      18.472  16.866  17.979  1.00 11.84      A    N
ATOM   2154  CA  GLY A 291      19.633  17.207  17.171  1.00 12.60      A    C
ATOM   2155  C   GLY A 291      19.466  18.506  16.400  1.00 12.44      A    C
ATOM   2156  O   GLY A 291      20.437  19.018  15.847  1.00 11.56      A    O
ATOM   2157  N   ALA A 292      18.249  19.056  16.378  1.00 12.96      A    N
ATOM   2158  CA  ALA A 292      17.960  20.238  15.562  1.00 13.11      A    C
ATOM   2159  CB  ALA A 292      16.454  20.468  15.434  1.00 12.99      A    C
ATOM   2160  C   ALA A 292      18.655  21.499  16.075  1.00 13.45      A    C
ATOM   2161  O   ALA A 292      18.954  21.612  17.252  1.00 13.95      A    O
ATOM   2162  N   ALA A 293      18.848  22.456  15.173  1.00 13.18      A    N
ATOM   2163  CA  ALA A 293      19.567  23.694  15.450  1.00 13.43      A    C
ATOM   2164  CB  ALA A 293      20.508  24.012  14.284  1.00 13.22      A    C
ATOM   2165  C   ALA A 293      18.611  24.866  15.637  1.00 13.54      A    C
ATOM   2166  O   ALA A 293      17.739  25.107  14.812  1.00 13.39      A    O
ATOM   2167  N   ASP A 294      18.838  25.626  16.691  1.00 13.60      A    N
ATOM   2168  CA  ASP A 294      18.167  26.895  16.899  1.00 14.04      A    C
ATOM   2169  CB  ASP A 294      18.590  27.428  18.270  1.00 14.33      A    C
ATOM   2170  CG  ASP A 294      17.918  28.728  18.634  1.00 14.83      A    C
ATOM   2171  OD1 ASP A 294      18.142  29.160  19.799  1.00 11.77      A    O
ATOM   2172  OD2 ASP A 294      17.144  29.360  17.861  1.00 10.92      A    O
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ATOM	2173	C	ASP	A	294	18.620	27.814	15.774	1.00	13.72	A	C
ATOM	2174	O	ASP	A	294	19.801	28.075	15.636	1.00	14.66	A	O
ATOM	2175	N	VAL	A	295	17.696	28.304	14.956	1.00	14.43	A	N
ATOM	2176	CA	VAL	A	295	18.057	29.217	13.853	1.00	14.05	A	C
ATOM	2177	CB	VAL	A	295	16.957	29.283	12.730	1.00	13.77	A	C
ATOM	2178	CG1	VAL	A	295	16.670	27.907	12.184	1.00	13.93	A	C
ATOM	2179	CG2	VAL	A	295	15.680	29.956	13.255	1.00	12.53	A	C
ATOM	2180	C	VAL	A	295	18.352	30.622	14.346	1.00	14.82	A	C
ATOM	2181	O	VAL	A	295	18.707	31.497	13.558	1.00	15.77	A	O
ATOM	2182	N	GLY	A	296	18.190	30.857	15.646	1.00	14.99	A	N
ATOM	2183	CA	GLY	A	296	18.450	32.159	16.208	1.00	15.10	A	C
ATOM	2184	C	GLY	A	296	17.282	32.821	16.906	1.00	15.03	A	C
ATOM	2185	O	GLY	A	296	17.458	33.886	17.489	1.00	15.00	A	O
ATOM	2186	N	LEU	A	297	16.114	32.180	16.887	1.00	16.05	A	N
ATOM	2187	CA	LEU	A	297	14.903	32.728	17.501	1.00	15.21	A	C
ATOM	2188	CB	LEU	A	297	13.704	32.420	16.605	1.00	14.95	A	C
ATOM	2189	CG	LEU	A	297	13.881	32.962	15.179	1.00	17.47	A	C
ATOM	2190	CD1	LEU	A	297	12.718	32.507	14.330	1.00	19.73	A	C
ATOM	2191	CD2	LEU	A	297	13.939	34.500	15.204	1.00	18.75	A	C
ATOM	2192	C	LEU	A	297	14.645	32.187	18.903	1.00	15.26	A	C
ATOM	2193	O	LEU	A	297	13.782	32.682	19.636	1.00	14.95	A	O
ATOM	2194	N	GLY	A	298	15.380	31.152	19.266	1.00	15.28	A	N
ATOM	2195	CA	GLY	A	298	15.251	30.546	20.570	1.00	15.27	A	C
ATOM	2196	C	GLY	A	298	14.024	29.691	20.721	1.00	15.55	A	C
ATOM	2197	O	GLY	A	298	13.173	29.572	19.817	1.00	15.07	A	O
ATOM	2198	N	PHE	A	299	13.941	29.090	21.894	1.00	15.47	A	N
ATOM	2199	CA	PHE	A	299	12.820	28.269	22.266	1.00	16.76	A	C
ATOM	2200	CB	PHE	A	299	13.279	26.818	22.539	1.00	16.33	A	C
ATOM	2201	CG	PHE	A	299	14.108	26.237	21.435	1.00	16.07	A	C
ATOM	2202	CD1	PHE	A	299	13.572	26.047	20.167	1.00	15.70	A	C
ATOM	2203	CE1	PHE	A	299	14.349	25.544	19.132	1.00	15.95	A	C
ATOM	2204	CZ	PHE	A	299	15.660	25.233	19.357	1.00	15.27	A	C
ATOM	2205	CE2	PHE	A	299	16.217	25.432	20.610	1.00	15.20	A	C
ATOM	2206	CD2	PHE	A	299	15.436	25.929	21.642	1.00	17.28	A	C
ATOM	2207	C	PHE	A	299	12.200	28.872	23.504	1.00	17.91	A	C
ATOM	2208	O	PHE	A	299	12.886	29.548	24.280	1.00	19.79	A	O
ATOM	2209	N	PRO	A	300	10.904	28.683	23.680	1.00	19.34	A	N
ATOM	2210	CA	PRO	A	300	10.054	27.945	22.747	1.00	20.29	A	C
ATOM	2211	CB	PRO	A	300	8.819	27.671	23.583	1.00	20.94	A	C
ATOM	2212	CG	PRO	A	300	8.712	28.898	24.513	1.00	19.43	A	C
ATOM	2213	CD	PRO	A	300	10.120	29.311	24.758	1.00	20.25	A	C
ATOM	2214	C	PRO	A	300	9.672	28.834	21.581	1.00	20.84	A	C
ATOM	2215	O	PRO	A	300	9.921	30.043	21.655	1.00	21.44	A	O
ATOM	2216	N	ASN	A	301	9.076	28.282	20.524	1.00	21.28	A	N
ATOM	2217	CA	ASN	A	301	8.874	29.078	19.319	1.00	21.53	A	C
ATOM	2218	CB	ASN	A	301	10.198	29.173	18.567	1.00	21.34	A	C
ATOM	2219	CG	ASN	A	301	10.320	30.458	17.764	1.00	20.14	A	C
ATOM	2220	OD1	ASN	A	301	9.875	30.553	16.607	1.00	17.42	A	O
ATOM	2221	ND2	ASN	A	301	10.920	31.454	18.371	1.00	22.84	A	N
ATOM	2222	C	ASN	A	301	7.823	28.534	18.355	1.00	22.14	A	C
ATOM	2223	O	ASN	A	301	7.868	27.379	17.978	1.00	23.49	A	O
ATOM	2224	N	GLY	A	302	6.970	29.416	17.854	1.00	22.24	A	N
ATOM	2225	CA	GLY	A	302	5.912	29.031	16.932	1.00	21.65	A	C
ATOM	2226	C	GLY	A	302	6.292	29.165	15.475	1.00	20.83	A	C
ATOM	2227	O	GLY	A	302	5.574	28.669	14.603	1.00	21.22	A	O
ATOM	2228	N	ASN	A	303	7.446	29.787	15.225	1.00	19.62	A	N
ATOM	2229	CA	ASN	A	303	7.981	30.005	13.886	1.00	17.66	A	C
ATOM	2230	CB	ASN	A	303	8.705	31.349	13.816	1.00	17.45	A	C

ATOM	2231	CG	ASN	A	303	7.872	32.473	14.381	1.00	20.84	A	C
ATOM	2232	OD1	ASN	A	303	6.802	32.779	13.847	1.00	21.34	A	O
ATOM	2233	ND2	ASN	A	303	8.305	33.033	15.530	1.00	22.58	A	N
ATOM	2234	C	ASN	A	303	8.926	28.922	13.414	1.00	15.61	A	C
ATOM	2235	O	ASN	A	303	8.831	28.481	12.239	1.00	13.70	A	O
ATOM	2236	N	GLN	A	304	9.841	28.506	14.298	1.00	14.18	A	N
ATOM	2237	CA	GLN	A	304	10.855	27.513	13.946	1.00	13.13	A	C
ATOM	2238	CB	GLN	A	304	12.235	28.005	14.316	1.00	13.28	A	C
ATOM	2239	CG	GLN	A	304	12.556	27.976	15.811	1.00	12.80	A	C
ATOM	2240	CD	GLN	A	304	14.020	28.087	16.123	1.00	11.63	A	C
ATOM	2241	OE1	GLN	A	304	14.842	27.582	15.386	1.00	13.19	A	O
ATOM	2242	NE2	GLN	A	304	14.352	28.794	17.223	1.00	9.76	A	N
ATOM	2243	C	GLN	A	304	10.601	26.128	14.582	1.00	13.52	A	C
ATOM	2244	O	GLN	A	304	11.372	25.208	14.381	1.00	13.66	A	O
ATOM	2245	N	GLY	A	305	9.537	25.972	15.343	1.00	12.81	A	N
ATOM	2246	CA	GLY	A	305	9.351	24.745	16.101	1.00	12.54	A	C
ATOM	2247	C	GLY	A	305	10.578	24.498	16.970	1.00	12.99	A	C
ATOM	2248	O	GLY	A	305	11.062	25.409	17.633	1.00	11.36	A	O
ATOM	2249	N	TRP	A	306	11.107	23.272	16.926	1.00	12.12	A	N
ATOM	2250	CA	TRP	A	306	12.286	22.898	17.701	1.00	12.07	A	C
ATOM	2251	CB	TRP	A	306	12.130	21.473	18.254	1.00	12.05	A	C
ATOM	2252	CG	TRP	A	306	10.866	21.349	19.092	1.00	11.34	A	C
ATOM	2253	CD1	TRP	A	306	9.755	20.611	18.805	1.00	12.28	A	C
ATOM	2254	NE1	TRP	A	306	8.812	20.766	19.794	1.00	13.42	A	N
ATOM	2255	CE2	TRP	A	306	9.316	21.592	20.761	1.00	12.23	A	C
ATOM	2256	CD2	TRP	A	306	10.616	21.963	20.359	1.00	13.78	A	C
ATOM	2257	CE3	TRP	A	306	11.344	22.822	21.183	1.00	13.41	A	C
ATOM	2258	CZ3	TRP	A	306	10.780	23.247	22.365	1.00	12.96	A	C
ATOM	2259	CH2	TRP	A	306	9.488	22.854	22.735	1.00	13.70	A	C
ATOM	2260	CZ2	TRP	A	306	8.744	22.035	21.945	1.00	14.65	A	C
ATOM	2261	C	TRP	A	306	13.562	23.046	16.890	1.00	12.73	A	C
ATOM	2262	O	TRP	A	306	14.632	22.620	17.318	1.00	14.46	A	O
ATOM	2263	N	GLY	A	307	13.479	23.716	15.741	1.00	13.10	A	N
ATOM	2264	CA	GLY	A	307	14.679	24.111	15.015	1.00	12.18	A	C
ATOM	2265	C	GLY	A	307	14.871	23.392	13.685	1.00	11.91	A	C
ATOM	2266	O	GLY	A	307	14.008	22.628	13.238	1.00	11.20	A	O
ATOM	2267	N	ARG	A	308	16.007	23.658	13.046	1.00	11.60	A	N
ATOM	2268	CA	ARG	A	308	16.299	23.167	11.701	1.00	12.01	A	C
ATOM	2269	CB	ARG	A	308	17.153	24.223	10.961	1.00	12.63	A	C
ATOM	2270	CG	ARG	A	308	17.388	23.970	9.462	1.00	13.43	A	C
ATOM	2271	CD	ARG	A	308	18.284	25.025	8.807	1.00	13.61	A	C
ATOM	2272	NE	ARG	A	308	19.563	25.031	9.510	1.00	16.45	A	N
ATOM	2273	CZ	ARG	A	308	20.127	26.086	10.086	1.00	16.43	A	C
ATOM	2274	NH1	ARG	A	308	21.257	25.902	10.762	1.00	14.45	A	N
ATOM	2275	NH2	ARG	A	308	19.660	27.319	9.902	1.00	13.23	A	N
ATOM	2276	C	ARG	A	308	17.055	21.837	11.770	1.00	12.38	A	C
ATOM	2277	O	ARG	A	308	18.094	21.742	12.434	1.00	12.82	A	O
ATOM	2278	N	VAL	A	309	16.549	20.817	11.080	1.00	11.99	A	N
ATOM	2279	CA	VAL	A	309	17.170	19.498	11.096	1.00	12.04	A	C
ATOM	2280	CB	VAL	A	309	16.553	18.573	10.051	1.00	11.35	A	C
ATOM	2281	CG1	VAL	A	309	17.354	17.272	9.961	1.00	11.45	A	C
ATOM	2282	CG2	VAL	A	309	15.047	18.335	10.377	1.00	11.38	A	C
ATOM	2283	C	VAL	A	309	18.667	19.545	10.868	1.00	12.28	A	C
ATOM	2284	O	VAL	A	309	19.148	20.157	9.930	1.00	11.94	A	O
ATOM	2285	N	THR	A	310	19.393	18.904	11.760	1.00	13.11	A	N
ATOM	2286	CA	THR	A	310	20.854	18.814	11.675	1.00	12.86	A	C
ATOM	2287	CB	THR	A	310	21.471	19.719	12.723	1.00	13.26	A	C
ATOM	2288	OG1	THR	A	310	21.044	21.090	12.516	1.00	12.98	A	O

ATOM	2289	CG2	THR	A	310	22.962	19.747	12.610	1.00	13.68	A	C
ATOM	2290	C	THR	A	310	21.197	17.347	11.911	1.00	13.94	A	C
ATOM	2291	O	THR	A	310	21.411	16.896	13.064	1.00	14.93	A	O
ATOM	2292	N	LEU	A	311	21.269	16.601	10.818	1.00	13.28	A	N
ATOM	2293	CA	LEU	A	311	21.110	15.149	10.879	1.00	14.11	A	C
ATOM	2294	CB	LEU	A	311	20.956	14.589	9.463	1.00	13.67	A	C
ATOM	2295	CG	LEU	A	311	20.879	13.078	9.311	1.00	13.50	A	C
ATOM	2296	CD1	LEU	A	311	19.749	12.522	10.109	1.00	15.11	A	C
ATOM	2297	CD2	LEU	A	311	20.749	12.688	7.849	1.00	14.22	A	C
ATOM	2298	C	LEU	A	311	22.252	14.455	11.605	1.00	14.58	A	C
ATOM	2299	O	LEU	A	311	22.012	13.521	12.345	1.00	14.74	A	O
ATOM	2300	N	ASP	A	312	23.483	14.959	11.462	1.00	15.58	A	N
ATOM	2301	CA	ASP	A	312	24.624	14.307	12.111	1.00	16.68	A	C
ATOM	2302	CB	ASP	A	312	25.984	14.797	11.582	1.00	16.93	A	C
ATOM	2303	CG	ASP	A	312	26.222	16.245	11.822	1.00	19.05	A	C
ATOM	2304	OD1	ASP	A	312	27.394	16.614	11.755	1.00	25.94	A	O
ATOM	2305	OD2	ASP	A	312	25.348	17.090	12.090	1.00	18.31	A	O
ATOM	2306	C	ASP	A	312	24.560	14.330	13.615	1.00	16.48	A	C
ATOM	2307	O	ASP	A	312	24.965	13.381	14.241	1.00	17.40	A	O
ATOM	2308	N	LYS	A	313	23.976	15.364	14.202	1.00	16.32	A	N
ATOM	2309	CA	LYS	A	313	23.755	15.366	15.641	1.00	16.35	A	C
ATOM	2310	CB	LYS	A	313	23.363	16.773	16.130	1.00	17.66	A	C
ATOM	2311	CG	LYS	A	313	24.430	17.848	15.938	1.00	20.65	A	C
ATOM	2312	CD	LYS	A	313	24.735	18.590	17.250	1.00	28.29	A	C
ATOM	2313	CE	LYS	A	313	25.619	17.746	18.162	1.00	31.10	A	C
ATOM	2314	NZ	LYS	A	313	26.458	18.529	19.131	1.00	32.31	A	N
ATOM	2315	C	LYS	A	313	22.666	14.379	16.100	1.00	15.36	A	C
ATOM	2316	O	LYS	A	313	22.662	13.968	17.258	1.00	15.49	A	O
ATOM	2317	N	SER	A	314	21.755	14.007	15.212	1.00	14.12	A	N
ATOM	2318	CA	SER	A	314	20.700	13.047	15.537	1.00	13.37	A	C
ATOM	2319	CB	SER	A	314	19.497	13.217	14.590	1.00	13.56	A	C
ATOM	2320	OG	SER	A	314	18.889	14.489	14.723	1.00	11.16	A	O
ATOM	2321	C	SER	A	314	21.148	11.581	15.505	1.00	14.53	A	C
ATOM	2322	O	SER	A	314	20.507	10.717	16.112	1.00	14.30	A	O
ATOM	2323	N	LEU	A	315	22.209	11.285	14.771	1.00	14.58	A	N
ATOM	2324	CA	LEU	A	315	22.563	9.896	14.484	1.00	15.64	A	C
ATOM	2325	CB	LEU	A	315	23.750	9.824	13.505	1.00	15.15	A	C
ATOM	2326	CG	LEU	A	315	23.506	10.436	12.143	1.00	14.88	A	C
ATOM	2327	CD1	LEU	A	315	24.834	10.445	11.360	1.00	16.67	A	C
ATOM	2328	CD2	LEU	A	315	22.401	9.683	11.411	1.00	16.28	A	C
ATOM	2329	C	LEU	A	315	22.905	9.095	15.733	1.00	16.16	A	C
ATOM	2330	O	LEU	A	315	22.442	7.956	15.894	1.00	16.79	A	O
ATOM	2331	N	ASN	A	316	23.692	9.686	16.631	1.00	17.60	A	N
ATOM	2332	CA	ASN	A	316	24.235	8.915	17.749	1.00	17.99	A	C
ATOM	2333	CB	ASN	A	316	25.757	8.837	17.694	1.00	19.59	A	C
ATOM	2334	CG	ASN	A	316	26.264	7.879	16.601	1.00	22.56	A	C
ATOM	2335	OD1	ASN	A	316	25.736	6.732	16.397	1.00	21.64	A	O
ATOM	2336	ND2	ASN	A	316	27.321	8.320	15.910	1.00	23.13	A	N
ATOM	2337	C	ASN	A	316	23.732	9.396	19.116	1.00	17.61	A	C
ATOM	2338	O	ASN	A	316	24.390	9.212	20.152	1.00	15.93	A	O
ATOM	2339	N	VAL	A	317	22.505	9.912	19.123	1.00	15.75	A	N
ATOM	2340	CA	VAL	A	317	21.820	10.220	20.389	1.00	15.40	A	C
ATOM	2341	CB	VAL	A	317	20.360	10.675	20.150	1.00	15.21	A	C
ATOM	2342	CG1	VAL	A	317	20.335	11.940	19.350	1.00	16.28	A	C
ATOM	2343	CG2	VAL	A	317	19.547	9.600	19.458	1.00	16.07	A	C
ATOM	2344	C	VAL	A	317	21.803	8.995	21.323	1.00	14.67	A	C
ATOM	2345	O	VAL	A	317	21.675	7.864	20.868	1.00	14.77	A	O
ATOM	2346	N	ALA	A	318	21.932	9.225	22.627	1.00	13.95	A	N

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ATOM   2347  CA  ALA A 318      21.623   8.186  23.603  1.00 13.64      A    C
ATOM   2348  CB  ALA A 318      22.196   8.523  24.940  1.00 13.50      A    C
ATOM   2349  C   ALA A 318      20.087   8.130  23.652  1.00 13.19      A    C
ATOM   2350  O   ALA A 318      19.416   9.168  23.498  1.00 13.46      A    O
ATOM   2351  N   PHE A 319      19.512   6.952  23.853  1.00 12.88      A    N
ATOM   2352  CA  PHE A 319      18.076   6.824  23.633  1.00 12.66      A    C
ATOM   2353  CB  PHE A 319      17.815   6.531  22.137  1.00 12.79      A    C
ATOM   2354  CG  PHE A 319      18.267   5.158  21.700  1.00 14.03      A    C
ATOM   2355  CD1 PHE A 319      19.504   4.980  21.107  1.00 12.44      A    C
ATOM   2356  CE1 PHE A 319      19.930   3.725  20.718  1.00 15.58      A    C
ATOM   2357  CZ  PHE A 319      19.115   2.619  20.921  1.00 15.26      A    C
ATOM   2358  CE2 PHE A 319      17.887   2.777  21.524  1.00 14.77      A    C
ATOM   2359  CD2 PHE A 319      17.461   4.047  21.905  1.00 15.05      A    C
ATOM   2360  C   PHE A 319      17.349   5.799  24.461  1.00 12.38      A    C
ATOM   2361  O   PHE A 319      17.947   4.918  25.055  1.00 12.11      A    O
ATOM   2362  N   VAL A 320      16.032   5.947  24.488  1.00 12.04      A    N
ATOM   2363  CA  VAL A 320      15.125   4.909  24.949  1.00 12.42      A    C
ATOM   2364  CB  VAL A 320      14.391   5.323  26.252  1.00 13.15      A    C
ATOM   2365  CG1 VAL A 320      13.237   4.331  26.589  1.00 13.46      A    C
ATOM   2366  CG2 VAL A 320      15.401   5.395  27.416  1.00 13.91      A    C
ATOM   2367  C   VAL A 320      14.137   4.758  23.802  1.00 11.88      A    C
ATOM   2368  O   VAL A 320      13.668   5.749  23.271  1.00 10.13      A    O
ATOM   2369  N   ASN A 321      13.824   3.520  23.441  1.00 11.82      A    N
ATOM   2370  CA  ASN A 321      13.018   3.205  22.261  1.00 11.75      A    C
ATOM   2371  CB  ASN A 321      13.858   2.323  21.313  1.00 11.75      A    C
ATOM   2372  CG  ASN A 321      13.214   2.117  19.944  1.00 12.10      A    C
ATOM   2373  OD1 ASN A 321      12.506   3.005  19.437  1.00 12.86      A    O
ATOM   2374  ND2 ASN A 321      13.451   0.919  19.328  1.00 10.43      A    N
ATOM   2375  C   ASN A 321      11.711   2.463  22.637  1.00 12.63      A    C
ATOM   2376  O   ASN A 321      11.509   1.311  22.260  1.00 12.41      A    O
ATOM   2377  N   GLU A 322      10.835   3.130  23.380  1.00 12.99      A    N
ATOM   2378  CA  GLU A 322       9.542   2.552  23.760  1.00 13.23      A    C
ATOM   2379  CB  GLU A 322       8.601   2.415  22.528  1.00 13.10      A    C
ATOM   2380  CG  GLU A 322       8.146   3.794  22.013  1.00 12.18      A    C
ATOM   2381  CD  GLU A 322       7.072   3.781  20.933  1.00 14.48      A    C
ATOM   2382  OE1 GLU A 322       6.747   4.884  20.429  1.00 15.20      A    O
ATOM   2383  OE2 GLU A 322       6.564   2.690  20.588  1.00 14.00      A    O
ATOM   2384  C   GLU A 322       9.654   1.239  24.556  1.00 14.04      A    C
ATOM   2385  O   GLU A 322       8.778   0.385  24.468  1.00 12.70      A    O
ATOM   2386  N   THR A 323      10.688   1.122  25.387  1.00 13.33      A    N
ATOM   2387  CA  THR A 323      10.907  -0.101  26.145  1.00 14.72      A    C
ATOM   2388  CB  THR A 323      12.375  -0.466  26.173  1.00 14.45      A    C
ATOM   2389  OG1 THR A 323      13.168   0.721  26.401  1.00 16.74      A    O
ATOM   2390  CG2 THR A 323      12.813  -0.980  24.810  1.00 15.39      A    C
ATOM   2391  C   THR A 323      10.397  -0.045  27.589  1.00 15.63      A    C
ATOM   2392  O   THR A 323      10.572  -1.011  28.319  1.00 14.71      A    O
ATOM   2393  N   SER A 324       9.796   1.073  28.002  1.00 15.41      A    N
ATOM   2394  CA  SER A 324       9.176   1.159  29.341  1.00 15.78      A    C
ATOM   2395  CB  SER A 324      10.008   2.045  30.272  1.00 15.94      A    C
ATOM   2396  OG  SER A 324      11.281   1.460  30.594  1.00 17.86      A    O
ATOM   2397  C   SER A 324       7.739   1.723  29.257  1.00 15.74      A    C
ATOM   2398  O   SER A 324       7.558   2.937  29.315  1.00 15.93      A    O
ATOM   2399  N   PRO A 325       6.729   0.864  29.118  1.00 16.08      A    N
ATOM   2400  CA  PRO A 325       5.326   1.306  29.170  1.00 17.17      A    C
ATOM   2401  CB  PRO A 325       4.525   0.035  28.823  1.00 17.76      A    C
ATOM   2402  CG  PRO A 325       5.454  -1.106  29.084  1.00 17.45      A    C
ATOM   2403  CD  PRO A 325       6.845  -0.585  28.885  1.00 16.38      A    C
ATOM   2404  C   PRO A 325       4.926   1.815  30.548  1.00 17.68      A    C
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ATOM   2405  O   PRO A 325       5.277   1.211  31.553  1.00 18.68      A    O
ATOM   2406  N   LEU A 326       4.204   2.916  30.596  1.00 18.30      A    N
ATOM   2407  CA  LEU A 326       3.796   3.491  31.871  1.00 18.53      A    C
ATOM   2408  CB  LEU A 326       4.410   4.890  32.059  1.00 18.37      A    C
ATOM   2409  CG  LEU A 326       5.938   5.027  32.161  1.00 19.30      A    C
ATOM   2410  CD1 LEU A 326       6.350   6.502  32.200  1.00 20.03      A    C
ATOM   2411  CD2 LEU A 326       6.471   4.338  33.387  1.00 17.55      A    C
ATOM   2412  C   LEU A 326       2.287   3.605  31.982  1.00 19.08      A    C
ATOM   2413  O   LEU A 326       1.589   3.926  30.989  1.00 18.42      A    O
ATOM   2414  N   SER A 327       1.810   3.326  33.201  1.00 19.13      A    N
ATOM   2415  CA  SER A 327       0.438   3.607  33.672  1.00 19.58      A    C
ATOM   2416  CB  SER A 327      -0.123   2.391  34.397  1.00 19.04      A    C
ATOM   2417  OG  SER A 327      -0.176   1.357  33.434  1.00 19.38      A    O
ATOM   2418  C   SER A 327       0.558   4.902  34.476  1.00 19.58      A    C
ATOM   2419  O   SER A 327       1.609   5.154  35.075  1.00 18.88      A    O
ATOM   2420  N   THR A 328      -0.505   5.696  34.595  1.00 20.38      A    N
ATOM   2421  CA  THR A 328      -0.861   6.454  35.789  1.00 19.96      A    C
ATOM   2422  CB  THR A 328      -2.343   6.678  35.951  1.00 20.43      A    C
ATOM   2423  OG1 THR A 328      -2.870   7.047  34.681  1.00 20.32      A    O
ATOM   2424  CG2 THR A 328      -2.602   7.922  36.842  1.00 21.84      A    C
ATOM   2425  C   THR A 328      -0.102   6.262  37.084  1.00 19.51      A    C
ATOM   2426  O   THR A 328      -0.223   5.222  37.739  1.00 19.59      A    O
ATOM   2427  N   SER A 329       0.732   7.268  37.356  1.00 18.40      A    N
ATOM   2428  CA  SER A 329       1.489   7.464  38.588  1.00 19.19      A    C
ATOM   2429  CB BSER A 329       0.679   7.017  39.818  0.50 19.34      A    C
ATOM   2430  CB ASER A 329       0.629   7.141  39.833  0.50 19.52      A    C
ATOM   2431  OG BSER A 329       0.653   5.599  39.887  0.50 18.73      A    O
ATOM   2432  OG ASER A 329      -0.672   7.722  39.718  0.50 20.52      A    O
ATOM   2433  C   SER A 329       2.792   6.686  38.588  1.00 18.71      A    C
ATOM   2434  O   SER A 329       3.533   6.753  39.550  1.00 18.11      A    O
ATOM   2435  N   GLN A 330       3.066   5.936  37.524  1.00 17.70      A    N
ATOM   2436  CA  GLN A 330       4.339   5.250  37.420  1.00 17.71      A    C
ATOM   2437  CB  GLN A 330       4.193   4.001  36.566  1.00 17.37      A    C
ATOM   2438  CG  GLN A 330       3.233   2.970  37.168  1.00 17.60      A    C
ATOM   2439  CD  GLN A 330       3.116   1.700  36.319  1.00 18.11      A    C
ATOM   2440  OE1 GLN A 330       3.305   1.763  35.119  1.00 16.08      A    O
ATOM   2441  NE2 GLN A 330       2.762   0.550  36.952  1.00 15.56      A    N
ATOM   2442  C   GLN A 330       5.401   6.195  36.837  1.00 18.14      A    C
ATOM   2443  O   GLN A 330       5.103   7.308  36.423  1.00 18.07      A    O
ATOM   2444  N   LYS A 331       6.643   5.750  36.842  1.00 18.66      A    N
ATOM   2445  CA  LYS A 331       7.710   6.524  36.276  1.00 19.23      A    C
ATOM   2446  CB  LYS A 331       8.229   7.550  37.289  1.00 20.19      A    C
ATOM   2447  CG  LYS A 331       8.972   6.934  38.450  1.00 23.65      A    C
ATOM   2448  CD  LYS A 331       9.071   7.912  39.625  1.00 28.70      A    C
ATOM   2449  CE  LYS A 331       9.954   7.332  40.754  1.00 31.64      A    C
ATOM   2450  NZ  LYS A 331      10.409   8.388  41.729  1.00 34.93      A    N
ATOM   2451  C   LYS A 331       8.804   5.589  35.820  1.00 18.87      A    C
ATOM   2452  O   LYS A 331       8.887   4.410  36.261  1.00 18.18      A    O
ATOM   2453  N   ALA A 332       9.587   6.091  34.873  1.00 17.37      A    N
ATOM   2454  CA  ALA A 332      10.797   5.406  34.412  1.00 17.82      A    C
ATOM   2455  CB  ALA A 332      10.689   5.068  32.941  1.00 17.06      A    C
ATOM   2456  C   ALA A 332      11.991   6.324  34.650  1.00 17.33      A    C
ATOM   2457  O   ALA A 332      11.999   7.480  34.213  1.00 16.52      A    O
ATOM   2458  N   THR A 333      13.005   5.805  35.325  1.00 17.85      A    N
ATOM   2459  CA  THR A 333      14.108   6.643  35.784  1.00 17.61      A    C
ATOM   2460  CB  THR A 333      14.194   6.544  37.304  1.00 18.03      A    C
ATOM   2461  OG1 THR A 333      12.956   6.966  37.902  1.00 19.93      A    O
ATOM   2462  CG2 THR A 333      15.234   7.490  37.851  1.00 18.18      A    C
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ATOM	2463	C	THR	A	333	15.410	6.186	35.159	1.00	17.36	A	C
ATOM	2464	O	THR	A	333	15.727	4.987	35.162	1.00	17.40	A	O
ATOM	2465	N	TYR	A	334	16.176	7.135	34.628	1.00	17.05	A	N
ATOM	2466	CA	TYR	A	334	17.437	6.840	33.986	1.00	17.42	A	C
ATOM	2467	CB	TYR	A	334	17.308	6.975	32.464	1.00	16.94	A	C
ATOM	2468	CG	TYR	A	334	16.144	6.230	31.860	1.00	16.41	A	C
ATOM	2469	CD1	TYR	A	334	16.273	4.891	31.458	1.00	14.43	A	C
ATOM	2470	CE1	TYR	A	334	15.205	4.205	30.912	1.00	14.63	A	C
ATOM	2471	CZ	TYR	A	334	13.977	4.846	30.772	1.00	15.02	A	C
ATOM	2472	OH	TYR	A	334	12.929	4.188	30.216	1.00	16.23	A	O
ATOM	2473	CE2	TYR	A	334	13.819	6.147	31.153	1.00	15.62	A	C
ATOM	2474	CD2	TYR	A	334	14.907	6.835	31.718	1.00	16.76	A	C
ATOM	2475	C	TYR	A	334	18.542	7.767	34.455	1.00	17.66	A	C
ATOM	2476	O	TYR	A	334	18.279	8.840	34.991	1.00	16.79	A	O
ATOM	2477	N	SER	A	335	19.783	7.375	34.169	1.00	17.44	A	N
ATOM	2478	CA	SER	A	335	20.939	8.218	34.442	1.00	18.62	A	C
ATOM	2479	CB	BSER	A	335	21.879	7.537	35.433	0.50	18.54	A	C
ATOM	2480	CB	ASER	A	335	21.916	7.518	35.393	0.50	18.59	A	C
ATOM	2481	OG	BSER	A	335	22.697	6.585	34.783	0.50	18.97	A	O
ATOM	2482	OG	ASER	A	335	21.316	7.174	36.629	0.50	19.43	A	O
ATOM	2483	C	SER	A	335	21.680	8.538	33.128	1.00	18.52	A	C
ATOM	2484	O	SER	A	335	21.698	7.720	32.221	1.00	18.14	A	O
ATOM	2485	N	PHE	A	336	22.298	9.715	33.049	1.00	17.92	A	N
ATOM	2486	CA	PHE	A	336	23.115	10.092	31.911	1.00	18.36	A	C
ATOM	2487	CB	PHE	A	336	22.324	10.949	30.900	1.00	18.52	A	C
ATOM	2488	CG	PHE	A	336	23.150	11.401	29.753	1.00	17.47	A	C
ATOM	2489	CD1	PHE	A	336	23.733	12.667	29.739	1.00	18.88	A	C
ATOM	2490	CE1	PHE	A	336	24.529	13.067	28.654	1.00	18.14	A	C
ATOM	2491	CZ	PHE	A	336	24.749	12.198	27.591	1.00	18.35	A	C
ATOM	2492	CE2	PHE	A	336	24.174	10.936	27.601	1.00	18.49	A	C
ATOM	2493	CD2	PHE	A	336	23.386	10.543	28.681	1.00	19.03	A	C
ATOM	2494	C	PHE	A	336	24.314	10.898	32.403	1.00	18.74	A	C
ATOM	2495	O	PHE	A	336	24.159	11.810	33.195	1.00	18.98	A	O
ATOM	2496	N	THR	A	337	25.504	10.547	31.938	1.00	19.28	A	N
ATOM	2497	CA	THR	A	337	26.733	11.219	32.364	1.00	19.77	A	C
ATOM	2498	CB	THR	A	337	27.879	10.201	32.343	1.00	20.11	A	C
ATOM	2499	OG1	THR	A	337	27.609	9.175	33.321	1.00	19.75	A	O
ATOM	2500	CG2	THR	A	337	29.159	10.857	32.796	1.00	21.58	A	C
ATOM	2501	C	THR	A	337	27.096	12.369	31.440	1.00	20.14	A	C
ATOM	2502	O	THR	A	337	27.266	12.163	30.253	1.00	20.10	A	O
ATOM	2503	N	ALA	A	338	27.181	13.571	32.000	1.00	19.74	A	N
ATOM	2504	CA	ALA	A	338	27.487	14.793	31.259	1.00	20.23	A	C
ATOM	2505	CB	ALA	A	338	26.468	15.858	31.588	1.00	19.43	A	C
ATOM	2506	C	ALA	A	338	28.881	15.292	31.633	1.00	20.94	A	C
ATOM	2507	O	ALA	A	338	29.389	14.991	32.710	1.00	19.43	A	O
ATOM	2508	N	GLN	A	339	29.503	16.042	30.741	1.00	22.51	A	N
ATOM	2509	CA	GLN	A	339	30.750	16.711	31.070	1.00	23.12	A	C
ATOM	2510	CB	GLN	A	339	31.893	16.162	30.230	1.00	24.34	A	C
ATOM	2511	CG	GLN	A	339	32.591	14.904	30.726	1.00	29.11	A	C
ATOM	2512	CD	GLN	A	339	34.116	14.923	30.437	1.00	36.99	A	C
ATOM	2513	OE1	GLN	A	339	34.841	13.991	30.825	1.00	41.39	A	O
ATOM	2514	NE2	GLN	A	339	34.597	15.995	29.778	1.00	36.90	A	N
ATOM	2515	C	GLN	A	339	30.543	18.167	30.722	1.00	23.27	A	C
ATOM	2516	O	GLN	A	339	30.034	18.485	29.641	1.00	23.02	A	O
ATOM	2517	N	ALA	A	340	30.922	19.061	31.619	1.00	22.60	A	N
ATOM	2518	CA	ALA	A	340	30.793	20.492	31.347	1.00	22.71	A	C
ATOM	2519	CB	ALA	A	340	31.311	21.296	32.535	1.00	22.84	A	C
ATOM	2520	C	ALA	A	340	31.524	20.916	30.076	1.00	22.30	A	C

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ATOM   2521  O   ALA A 340      32.474  20.270  29.650  1.00 22.44      A    O
ATOM   2522  N   GLY A 341      31.063  21.996  29.455  1.00 23.38      A    N
ATOM   2523  CA  GLY A 341      31.738  22.554  28.283  1.00 23.73      A    C
ATOM   2524  C   GLY A 341      30.989  22.425  26.956  1.00 24.15      A    C
ATOM   2525  O   GLY A 341      31.457  22.902  25.917  1.00 24.10      A    O
ATOM   2526  N   LYS A 342      29.829  21.774  26.970  1.00 24.05      A    N
ATOM   2527  CA  LYS A 342      29.038  21.637  25.743  1.00 24.39      A    C
ATOM   2528  CB  LYS A 342      29.643  20.545  24.861  1.00 25.08      A    C
ATOM   2529  CG  LYS A 342      29.610  19.148  25.496  1.00 27.13      A    C
ATOM   2530  CD  LYS A 342      30.471  18.173  24.723  1.00 29.40      A    C
ATOM   2531  CE  LYS A 342      30.254  16.725  25.182  1.00 29.96      A    C
ATOM   2532  NZ  LYS A 342      30.738  16.515  26.576  1.00 32.09      A    N
ATOM   2533  C   LYS A 342      27.552  21.373  26.058  1.00 23.40      A    C
ATOM   2534  O   LYS A 342      27.220  20.861  27.144  1.00 23.54      A    O
ATOM   2535  N   PRO A 343      26.652  21.755  25.151  1.00 22.09      A    N
ATOM   2536  CA  PRO A 343      25.219  21.683  25.450  1.00 21.01      A    C
ATOM   2537  CB  PRO A 343      24.557  22.206  24.163  1.00 21.58      A    C
ATOM   2538  CG  PRO A 343      25.613  23.026  23.492  1.00 22.06      A    C
ATOM   2539  CD  PRO A 343      26.902  22.348  23.820  1.00 22.30      A    C
ATOM   2540  C   PRO A 343      24.729  20.279  25.756  1.00 19.35      A    C
ATOM   2541  O   PRO A 343      25.311  19.298  25.317  1.00 17.82      A    O
ATOM   2542  N   LEU A 344      23.645  20.223  26.521  1.00 18.12      A    N
ATOM   2543  CA  LEU A 344      22.945  18.988  26.790  1.00 17.07      A    C
ATOM   2544  CB  LEU A 344      23.019  18.680  28.278  1.00 17.12      A    C
ATOM   2545  CG  LEU A 344      22.250  17.476  28.788  1.00 16.96      A    C
ATOM   2546  CD1 LEU A 344      22.743  16.188  28.128  1.00 16.29      A    C
ATOM   2547  CD2 LEU A 344      22.399  17.414  30.336  1.00 17.28      A    C
ATOM   2548  C   LEU A 344      21.484  19.168  26.360  1.00 16.41      A    C
ATOM   2549  O   LEU A 344      20.814  20.029  26.870  1.00 17.49      A    O
ATOM   2550  N   LYS A 345      21.013  18.336  25.440  1.00 15.23      A    N
ATOM   2551  CA  LYS A 345      19.638  18.405  24.943  1.00 14.51      A    C
ATOM   2552  CB  LYS A 345      19.644  18.807  23.474  1.00 14.84      A    C
ATOM   2553  CG  LYS A 345      20.104  20.235  23.248  1.00 13.82      A    C
ATOM   2554  CD  LYS A 345      19.987  20.664  21.795  1.00 16.32      A    C
ATOM   2555  CE  LYS A 345      18.599  21.126  21.423  1.00 13.96      A    C
ATOM   2556  NZ  LYS A 345      18.513  21.491  19.992  1.00 17.70      A    N
ATOM   2557  C   LYS A 345      18.929  17.066  25.135  1.00 14.25      A    C
ATOM   2558  O   LYS A 345      19.399  16.033  24.658  1.00 14.33      A    O
ATOM   2559  N   ILE A 346      17.821  17.084  25.870  1.00 13.41      A    N
ATOM   2560  CA  ILE A 346      17.031  15.888  26.116  1.00 13.30      A    C
ATOM   2561  CB  ILE A 346      16.983  15.589  27.619  1.00 13.25      A    C
ATOM   2562  CG1 ILE A 346      18.376  15.444  28.197  1.00 13.74      A    C
ATOM   2563  CD1 ILE A 346      18.459  15.807  29.637  1.00 15.75      A    C
ATOM   2564  CG2 ILE A 346      16.180  14.329  27.874  1.00 13.54      A    C
ATOM   2565  C   ILE A 346      15.598  16.084  25.601  1.00 13.26      A    C
ATOM   2566  O   ILE A 346      14.900  17.010  26.020  1.00 13.15      A    O
ATOM   2567  N   SER A 347      15.159  15.197  24.714  1.00 12.65      A    N
ATOM   2568  CA  SER A 347      13.795  15.262  24.172  1.00 12.47      A    C
ATOM   2569  CB BSER A 347      13.838  15.473  22.654  0.35 12.36      A    C
ATOM   2570  CB ASER A 347      13.813  15.524  22.662  0.65 12.73      A    C
ATOM   2571  OG BSER A 347      12.569  15.297  22.042  0.35 10.59      A    O
ATOM   2572  OG ASER A 347      14.655  16.634  22.329  0.65 13.18      A    O
ATOM   2573  C   SER A 347      13.032  13.983  24.491  1.00 11.72      A    C
ATOM   2574  O   SER A 347      13.511  12.881  24.219  1.00 11.81      A    O
ATOM   2575  N   LEU A 348      11.830  14.165  25.026  1.00 11.03      A    N
ATOM   2576  CA  LEU A 348      10.864  13.121  25.289  1.00 10.93      A    C
ATOM   2577  CB  LEU A 348      10.302  13.274  26.706  1.00 10.96      A    C
ATOM   2578  CG  LEU A 348       9.054  12.502  27.097  1.00 10.80      A    C
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ATOM   2579  CD1 LEU A 348       9.396  11.029  27.180  1.00 13.05      A    C
ATOM   2580  CD2 LEU A 348       8.542  12.969  28.443  1.00 12.50      A    C
ATOM   2581  C   LEU A 348       9.735  13.231  24.287  1.00 11.09      A    C
ATOM   2582  O   LEU A 348       9.152  14.302  24.140  1.00 12.01      A    O
ATOM   2583  N   VAL A 349       9.389  12.127  23.631  1.00 10.58      A    N
ATOM   2584  CA  VAL A 349       8.327  12.142  22.638  1.00 11.32      A    C
ATOM   2585  CB  VAL A 349       8.876  12.223  21.185  1.00 11.27      A    C
ATOM   2586  CG1 VAL A 349       7.745  12.102  20.169  1.00 12.19      A    C
ATOM   2587  CG2 VAL A 349       9.653  13.511  20.961  1.00 11.93      A    C
ATOM   2588  C   VAL A 349       7.522  10.873  22.768  1.00 11.68      A    C
ATOM   2589  O   VAL A 349       8.099   9.802  22.870  1.00 12.43      A    O
ATOM   2590  N   TRP A 350       6.200  10.993  22.768  1.00 11.69      A    N
ATOM   2591  CA  TRP A 350       5.354   9.813  22.662  1.00 11.48      A    C
ATOM   2592  CB  TRP A 350       4.719   9.442  24.002  1.00 11.79      A    C
ATOM   2593  CG  TRP A 350       3.822  10.448  24.628  1.00 11.11      A    C
ATOM   2594  CD1 TRP A 350       2.457  10.378  24.720  1.00 12.11      A    C
ATOM   2595  NE1 TRP A 350       1.961  11.469  25.386  1.00 12.24      A    N
ATOM   2596  CE2 TRP A 350       3.015  12.262  25.774  1.00 13.16      A    C
ATOM   2597  CD2 TRP A 350       4.208  11.640  25.311  1.00 13.33      A    C
ATOM   2598  CE3 TRP A 350       5.440  12.249  25.593  1.00 12.51      A    C
ATOM   2599  CZ3 TRP A 350       5.444  13.449  26.311  1.00 13.31      A    C
ATOM   2600  CH2 TRP A 350       4.248  14.022  26.767  1.00 13.75      A    C
ATOM   2601  CZ2 TRP A 350       3.022  13.427  26.507  1.00 13.59      A    C
ATOM   2602  C   TRP A 350       4.314   9.883  21.536  1.00 11.50      A    C
ATOM   2603  O   TRP A 350       3.905  10.953  21.077  1.00 11.90      A    O
ATOM   2604  N   SER A 351       3.921   8.707  21.071  1.00 11.83      A    N
ATOM   2605  CA  SER A 351       2.889   8.607  20.070  1.00 12.20      A    C
ATOM   2606  CB  SER A 351       3.182   7.496  19.070  1.00 12.11      A    C
ATOM   2607  OG  SER A 351       4.356   7.772  18.310  1.00 11.85      A    O
ATOM   2608  C   SER A 351       1.636   8.378  20.884  1.00 12.65      A    C
ATOM   2609  O   SER A 351       1.360   7.285  21.375  1.00 12.72      A    O
ATOM   2610  N   ASP A 352       0.947   9.477  21.115  1.00 13.75      A    N
ATOM   2611  CA  ASP A 352      -0.205   9.532  21.982  1.00 14.48      A    C
ATOM   2612  CB  ASP A 352      -0.508  11.003  22.225  1.00 14.84      A    C
ATOM   2613  CG  ASP A 352      -1.480  11.251  23.385  1.00 16.70      A    C
ATOM   2614  OD1 ASP A 352      -1.655  10.366  24.260  1.00 15.50      A    O
ATOM   2615  OD2 ASP A 352      -2.115  12.329  23.458  1.00 15.19      A    O
ATOM   2616  C   ASP A 352      -1.427   8.842  21.389  1.00 15.19      A    C
ATOM   2617  O   ASP A 352      -1.569   8.678  20.155  1.00 15.52      A    O
ATOM   2618  N   ALA A 353      -2.331   8.434  22.273  1.00 15.26      A    N
ATOM   2619  CA  ALA A 353      -3.689   8.074  21.853  1.00 15.65      A    C
ATOM   2620  CB  ALA A 353      -4.526   7.801  23.051  1.00 15.59      A    C
ATOM   2621  C   ALA A 353      -4.325   9.197  21.018  1.00 15.42      A    C
ATOM   2622  O   ALA A 353      -4.076  10.374  21.264  1.00 15.11      A    O
ATOM   2623  N   PRO A 354      -5.157   8.840  20.041  1.00 16.50      A    N
ATOM   2624  CA  PRO A 354      -5.858   9.841  19.235  1.00 16.92      A    C
ATOM   2625  CB  PRO A 354      -6.724   9.003  18.287  1.00 17.36      A    C
ATOM   2626  CG  PRO A 354      -6.790   7.646  18.897  1.00 17.45      A    C
ATOM   2627  CD  PRO A 354      -5.499   7.456  19.640  1.00 16.81      A    C
ATOM   2628  C   PRO A 354      -6.723  10.771  20.073  1.00 18.05      A    C
ATOM   2629  O   PRO A 354      -7.420  10.293  20.957  1.00 17.51      A    O
ATOM   2630  N   GLY A 355      -6.629  12.074  19.819  1.00 18.60      A    N
ATOM   2631  CA  GLY A 355      -7.392  13.071  20.527  1.00 20.06      A    C
ATOM   2632  C   GLY A 355      -8.773  13.285  19.936  1.00 21.21      A    C
ATOM   2633  O   GLY A 355      -9.095  12.758  18.880  1.00 22.41      A    O
ATOM   2634  N   SER A 356      -9.598  14.050  20.628  1.00 22.87      A    N
ATOM   2635  CA  SER A 356     -10.939  14.377  20.145  1.00 23.97      A    C
ATOM   2636  CB  SER A 356     -11.924  14.555  21.319  1.00 24.97      A    C
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ATOM   2637  OG  SER A 356     -12.771  15.696  21.117  1.00 26.85      A    O
ATOM   2638  C   SER A 356     -10.901  15.654  19.320  1.00 24.04      A    C
ATOM   2639  O   SER A 356     -10.151  16.583  19.635  1.00 23.54      A    O
ATOM   2640  N   THR A 357     -11.714  15.684  18.261  1.00 24.61      A    N
ATOM   2641  CA  THR A 357     -11.826  16.846  17.396  1.00 25.58      A    C
ATOM   2642  CB  THR A 357     -12.423  16.436  16.032  1.00 25.86      A    C
ATOM   2643  OG1 THR A 357     -13.673  15.748  16.218  1.00 25.91      A    O
ATOM   2644  CG2 THR A 357     -11.534  15.392  15.334  1.00 25.30      A    C
ATOM   2645  C   THR A 357     -12.687  17.982  18.000  1.00 26.58      A    C
ATOM   2646  O   THR A 357     -12.812  19.035  17.398  1.00 26.22      A    O
ATOM   2647  N   THR A 358     -13.276  17.771  19.175  1.00 27.59      A    N
ATOM   2648  CA  THR A 358     -14.113  18.816  19.779  1.00 28.37      A    C
ATOM   2649  CB  THR A 358     -15.575  18.335  19.938  1.00 28.27      A    C
ATOM   2650  OG1 THR A 358     -15.606  17.065  20.606  1.00 28.60      A    O
ATOM   2651  CG2 THR A 358     -16.192  18.066  18.587  1.00 27.97      A    C
ATOM   2652  C   THR A 358     -13.605  19.321  21.118  1.00 28.71      A    C
ATOM   2653  O   THR A 358     -13.954  20.424  21.524  1.00 29.22      A    O
ATOM   2654  N   ALA A 359     -12.758  18.548  21.795  1.00 28.63      A    N
ATOM   2655  CA  ALA A 359     -12.311  18.925  23.133  1.00 27.94      A    C
ATOM   2656  CB  ALA A 359     -11.668  17.739  23.814  1.00 28.64      A    C
ATOM   2657  C   ALA A 359     -11.349  20.100  23.099  1.00 27.98      A    C
ATOM   2658  O   ALA A 359     -10.738  20.393  22.060  1.00 27.61      A    O
ATOM   2659  N   SER A 360     -11.213  20.785  24.241  1.00 27.18      A    N
ATOM   2660  CA  SER A 360     -10.301  21.916  24.344  1.00 27.00      A    C
ATOM   2661  CB  SER A 360     -10.351  22.564  25.737  1.00 27.57      A    C
ATOM   2662  OG  SER A 360     -11.688  22.840  26.125  1.00 31.54      A    O
ATOM   2663  C   SER A 360      -8.858  21.485  24.060  1.00 25.14      A    C
ATOM   2664  O   SER A 360      -8.115  22.230  23.446  1.00 24.27      A    O
ATOM   2665  N   LEU A 361      -8.478  20.307  24.553  1.00 23.74      A    N
ATOM   2666  CA  LEU A 361      -7.100  19.812  24.453  1.00 23.54      A    C
ATOM   2667  CB  LEU A 361      -6.480  19.583  25.840  1.00 23.87      A    C
ATOM   2668  CG  LEU A 361      -6.119  20.802  26.702  1.00 27.30      A    C
ATOM   2669  CD1 LEU A 361      -5.434  20.335  27.980  1.00 28.61      A    C
ATOM   2670  CD2 LEU A 361      -5.217  21.827  25.975  1.00 28.84      A    C
ATOM   2671  C   LEU A 361      -7.097  18.493  23.701  1.00 21.78      A    C
ATOM   2672  O   LEU A 361      -7.942  17.611  23.961  1.00 21.73      A    O
ATOM   2673  N   THR A 362      -6.141  18.325  22.790  1.00 19.81      A    N
ATOM   2674  CA  THR A 362      -6.053  17.058  22.066  1.00 18.76      A    C
ATOM   2675  CB  THR A 362      -5.433  17.230  20.657  1.00 19.42      A    C
ATOM   2676  OG1 THR A 362      -4.100  17.707  20.786  1.00 17.51      A    O
ATOM   2677  CG2 THR A 362      -6.174  18.305  19.862  1.00 20.58      A    C
ATOM   2678  C   THR A 362      -5.261  16.023  22.819  1.00 17.21      A    C
ATOM   2679  O   THR A 362      -5.411  14.858  22.530  1.00 13.79      A    O
ATOM   2680  N   LEU A 363      -4.398  16.448  23.761  1.00 16.68      A    N
ATOM   2681  CA  LEU A 363      -3.560  15.505  24.484  1.00 16.39      A    C
ATOM   2682  CB  LEU A 363      -2.547  16.213  25.411  1.00 16.30      A    C
ATOM   2683  CG  LEU A 363      -1.460  15.318  25.990  1.00 16.62      A    C
ATOM   2684  CD1 LEU A 363      -0.380  14.960  24.939  1.00 16.31      A    C
ATOM   2685  CD2 LEU A 363      -0.838  15.936  27.236  1.00 15.84      A    C
ATOM   2686  C   LEU A 363      -4.424  14.536  25.280  1.00 17.11      A    C
ATOM   2687  O   LEU A 363      -5.404  14.936  25.911  1.00 17.15      A    O
ATOM   2688  N   VAL A 364      -4.068  13.253  25.249  1.00 16.50      A    N
ATOM   2689  CA  VAL A 364      -4.829  12.263  25.975  1.00 16.09      A    C
ATOM   2690  CB  VAL A 364      -5.285  11.121  25.030  1.00 15.79      A    C
ATOM   2691  CG1 VAL A 364      -5.871   9.933  25.826  1.00 17.24      A    C
ATOM   2692  CG2 VAL A 364      -6.288  11.651  24.020  1.00 16.26      A    C
ATOM   2693  C   VAL A 364      -3.983  11.744  27.139  1.00 15.68      A    C
ATOM   2694  O   VAL A 364      -4.329  11.942  28.309  1.00 15.17      A    O
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ATOM   2695  N   ASN A 365      -2.875  11.085  26.809  1.00 14.41      A    N
ATOM   2696  CA  ASN A 365      -1.931  10.614  27.804  1.00 14.31      A    C
ATOM   2697  CB  ASN A 365      -1.302   9.286  27.354  1.00 14.31      A    C
ATOM   2698  CG  ASN A 365      -2.342   8.161  27.214  1.00 16.21      A    C
ATOM   2699  OD1 ASN A 365      -3.298   8.081  28.004  1.00 13.31      A    O
ATOM   2700  ND2 ASN A 365      -2.158   7.283  26.206  1.00 14.49      A    N
ATOM   2701  C   ASN A 365      -0.858  11.690  28.088  1.00 14.80      A    C
ATOM   2702  O   ASN A 365      -0.174  12.190  27.172  1.00 14.01      A    O
ATOM   2703  N   ASP A 366      -0.696  12.015  29.360  1.00 14.06      A    N
ATOM   2704  CA  ASP A 366       0.158  13.115  29.783  1.00 15.00      A    C
ATOM   2705  CB  ASP A 366      -0.632  14.068  30.672  1.00 14.40      A    C
ATOM   2706  CG  ASP A 366       0.105  15.346  30.990  1.00 15.13      A    C
ATOM   2707  OD1 ASP A 366       1.344  15.467  30.710  1.00 13.15      A    O
ATOM   2708  OD2 ASP A 366      -0.491  16.284  31.609  1.00 17.79      A    O
ATOM   2709  C   ASP A 366       1.367  12.568  30.548  1.00 14.89      A    C
ATOM   2710  O   ASP A 366       1.257  12.132  31.708  1.00 15.57      A    O
ATOM   2711  N   LEU A 367       2.501  12.562  29.865  1.00 14.16      A    N
ATOM   2712  CA  LEU A 367       3.772  12.248  30.462  1.00 14.65      A    C
ATOM   2713  CB  LEU A 367       4.581  11.333  29.520  1.00 14.37      A    C
ATOM   2714  CG  LEU A 367       3.990  10.005  29.077  1.00 13.06      A    C
ATOM   2715  CD1 LEU A 367       5.063   9.220  28.244  1.00 12.20      A    C
ATOM   2716  CD2 LEU A 367       3.485   9.123  30.239  1.00 15.25      A    C
ATOM   2717  C   LEU A 367       4.523  13.555  30.710  1.00 14.15      A    C
ATOM   2718  O   LEU A 367       4.271  14.546  30.045  1.00 14.17      A    O
ATOM   2719  N   ASP A 368       5.441  13.556  31.677  1.00 14.04      A    N
ATOM   2720  CA  ASP A 368       6.271  14.705  31.980  1.00 14.28      A    C
ATOM   2721  CB  ASP A 368       5.959  15.284  33.354  1.00 15.52      A    C
ATOM   2722  CG  ASP A 368       4.529  15.726  33.515  1.00 17.54      A    C
ATOM   2723  OD1 ASP A 368       3.909  16.253  32.540  1.00 14.48      A    O
ATOM   2724  OD2 ASP A 368       4.006  15.624  34.642  1.00 17.39      A    O
ATOM   2725  C   ASP A 368       7.724  14.275  32.057  1.00 14.49      A    C
ATOM   2726  O   ASP A 368       8.034  13.203  32.587  1.00 13.94      A    O
ATOM   2727  N   LEU A 369       8.603  15.108  31.520  1.00 14.32      A    N
ATOM   2728  CA  LEU A 369      10.044  14.937  31.645  1.00 14.31      A    C
ATOM   2729  CB  LEU A 369      10.735  15.448  30.380  1.00 13.72      A    C
ATOM   2730  CG  LEU A 369      12.238  15.284  30.298  1.00 12.96      A    C
ATOM   2731  CD1 LEU A 369      12.572  13.850  30.345  1.00 12.52      A    C
ATOM   2732  CD2 LEU A 369      12.749  15.953  28.980  1.00 14.11      A    C
ATOM   2733  C   LEU A 369      10.539  15.733  32.854  1.00 15.02      A    C
ATOM   2734  O   LEU A 369      10.218  16.922  33.012  1.00 15.50      A    O
ATOM   2735  N   VAL A 370      11.315  15.085  33.698  1.00 15.26      A    N
ATOM   2736  CA  VAL A 370      11.875  15.729  34.905  1.00 15.63      A    C
ATOM   2737  CB  VAL A 370      11.144  15.278  36.180  1.00 15.95      A    C
ATOM   2738  CG1 VAL A 370      11.679  16.020  37.425  1.00 17.73      A    C
ATOM   2739  CG2 VAL A 370       9.687  15.487  36.024  1.00 15.57      A    C
ATOM   2740  C   VAL A 370      13.359  15.388  34.975  1.00 15.46      A    C
ATOM   2741  O   VAL A 370      13.767  14.219  35.042  1.00 15.96      A    O
ATOM   2742  N   ILE A 371      14.174  16.422  34.908  1.00 15.15      A    N
ATOM   2743  CA  ILE A 371      15.608  16.261  34.858  1.00 14.98      A    C
ATOM   2744  CB  ILE A 371      16.171  17.036  33.669  1.00 14.71      A    C
ATOM   2745  CG1 ILE A 371      15.509  16.589  32.336  1.00 14.63      A    C
ATOM   2746  CD1 ILE A 371      15.600  15.075  32.072  1.00 14.66      A    C
ATOM   2747  CG2 ILE A 371      17.674  16.922  33.614  1.00 12.85      A    C
ATOM   2748  C   ILE A 371      16.145  16.835  36.155  1.00 15.95      A    C
ATOM   2749  O   ILE A 371      15.648  17.853  36.618  1.00 16.74      A    O
ATOM   2750  N   THR A 372      17.150  16.174  36.727  1.00 16.86      A    N
ATOM   2751  CA  THR A 372      17.858  16.671  37.897  1.00 17.19      A    C
ATOM   2752  CB  THR A 372      17.618  15.748  39.089  1.00 17.36      A    C
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ATOM	2753	OG1	THR	A	372	16.212	15.514	39.265	1.00	18.17	A	O
ATOM	2754	CG2	THR	A	372	18.044	16.409	40.372	1.00	17.84	A	C
ATOM	2755	C	THR	A	372	19.364	16.729	37.634	1.00	17.65	A	C
ATOM	2756	O	THR	A	372	19.962	15.725	37.262	1.00	18.44	A	O
ATOM	2757	N	ALA	A	373	19.971	17.891	37.870	1.00	17.80	A	N
ATOM	2758	CA	ALA	A	373	21.376	18.118	37.606	1.00	18.13	A	C
ATOM	2759	CB	ALA	A	373	21.643	19.607	37.475	1.00	18.43	A	C
ATOM	2760	C	ALA	A	373	22.175	17.545	38.767	1.00	19.16	A	C
ATOM	2761	O	ALA	A	373	21.601	17.188	39.780	1.00	18.57	A	O
ATOM	2762	N	PRO	A	374	23.479	17.368	38.581	1.00	19.84	A	N
ATOM	2763	CA	PRO	A	374	24.348	16.857	39.642	1.00	20.99	A	C
ATOM	2764	CB	PRO	A	374	25.727	16.884	39.001	1.00	20.60	A	C
ATOM	2765	CG	PRO	A	374	25.434	16.700	37.530	1.00	20.96	A	C
ATOM	2766	CD	PRO	A	374	24.174	17.460	37.286	1.00	20.29	A	C
ATOM	2767	C	PRO	A	374	24.266	17.647	40.948	1.00	22.06	A	C
ATOM	2768	O	PRO	A	374	24.303	17.039	42.011	1.00	23.95	A	O
ATOM	2769	N	ASN	A	375	24.024	18.954	40.873	1.00	23.03	A	N
ATOM	2770	CA	ASN	A	375	23.910	19.770	42.058	1.00	23.32	A	C
ATOM	2771	CB	ASN	A	375	24.515	21.165	41.790	1.00	24.03	A	C
ATOM	2772	CG	ASN	A	375	23.581	22.096	40.993	1.00	26.93	A	C
ATOM	2773	OD1	ASN	A	375	22.515	21.689	40.492	1.00	28.51	A	O
ATOM	2774	ND2	ASN	A	375	23.987	23.362	40.878	1.00	27.28	A	N
ATOM	2775	C	ASN	A	375	22.471	19.898	42.563	1.00	23.07	A	C
ATOM	2776	O	ASN	A	375	22.208	20.711	43.430	1.00	22.92	A	O
ATOM	2777	N	GLY	A	376	21.541	19.120	42.010	1.00	21.76	A	N
ATOM	2778	CA	GLY	A	376	20.166	19.165	42.469	1.00	21.43	A	C
ATOM	2779	C	GLY	A	376	19.197	20.077	41.724	1.00	20.91	A	C
ATOM	2780	O	GLY	A	376	17.990	20.006	41.937	1.00	19.94	A	O
ATOM	2781	N	THR	A	377	19.696	20.909	40.828	1.00	21.29	A	N
ATOM	2782	CA	THR	A	377	18.793	21.785	40.090	1.00	21.36	A	C
ATOM	2783	CB	THR	A	377	19.571	22.738	39.220	1.00	21.19	A	C
ATOM	2784	OG1	THR	A	377	20.423	23.532	40.054	1.00	22.26	A	O
ATOM	2785	CG2	THR	A	377	18.635	23.724	38.538	1.00	20.97	A	C
ATOM	2786	C	THR	A	377	17.818	20.971	39.239	1.00	20.56	A	C
ATOM	2787	O	THR	A	377	18.206	20.058	38.541	1.00	19.93	A	O
ATOM	2788	N	LYS	A	378	16.558	21.345	39.315	1.00	20.68	A	N
ATOM	2789	CA	LYS	A	378	15.488	20.630	38.644	1.00	21.64	A	C
ATOM	2790	CB	LYS	A	378	14.321	20.503	39.594	1.00	22.42	A	C
ATOM	2791	CG	LYS	A	378	13.709	19.168	39.611	1.00	28.13	A	C
ATOM	2792	CD	LYS	A	378	14.144	18.449	40.913	1.00	33.32	A	C
ATOM	2793	CE	LYS	A	378	13.743	17.001	40.854	1.00	34.92	A	C
ATOM	2794	NZ	LYS	A	378	14.605	16:111	41.699	1.00	38.61	A	N
ATOM	2795	C	LYS	A	378	14.990	21.344	37.397	1.00	20.06	A	C
ATOM	2796	O	LYS	A	378	14.902	22.553	37.388	1.00	19.59	A	O
ATOM	2797	N	TYR	A	379	14.623	20.568	36.378	1.00	18.59	A	N
ATOM	2798	CA	TYR	A	379	14.009	21.088	35.155	1.00	17.87	A	C
ATOM	2799	CB	TYR	A	379	15.030	21.111	34.011	1.00	17.25	A	C
ATOM	2800	CG	TYR	A	379	16.382	21.654	34.386	1.00	17.53	A	C
ATOM	2801	CD1	TYR	A	379	17.297	20.864	35.052	1.00	18.58	A	C
ATOM	2802	CE1	TYR	A	379	18.537	21.352	35.417	1.00	19.05	A	C
ATOM	2803	CZ	TYR	A	379	18.895	22.655	35.097	1.00	21.25	A	C
ATOM	2804	OH	TYR	A	379	20.160	23.104	35.465	1.00	20.46	A	O
ATOM	2805	CE2	TYR	A	379	18.004	23.459	34.399	1.00	19.58	A	C
ATOM	2806	CD2	TYR	A	379	16.751	22.953	34.060	1.00	18.07	A	C
ATOM	2807	C	TYR	A	379	12.852	20.198	34.732	1.00	17.42	A	C
ATOM	2808	O	TYR	A	379	12.967	18.973	34.766	1.00	18.13	A	O
ATOM	2809	N	VAL	A	380	11.732	20.787	34.340	1.00	16.44	A	N
ATOM	2810	CA	VAL	A	380	10.653	19.989	33.750	1.00	16.11	A	C

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ATOM   2811  CB  VAL A 380       9.320  20.114  34.514  1.00 16.66      A    C
ATOM   2812  CG1 VAL A 380       9.521  19.742  36.000  1.00 17.64      A    C
ATOM   2813  CG2 VAL A 380       8.716  21.505  34.369  1.00 16.52      A    C
ATOM   2814  C   VAL A 380      10.466  20.353  32.283  1.00 14.93      A    C
ATOM   2815  O   VAL A 380      10.876  21.425  31.826  1.00 15.17      A    O
ATOM   2816  N   GLY A 381       9.868  19.436  31.547  1.00 14.19      A    N
ATOM   2817  CA  GLY A 381       9.761  19.541  30.101  1.00 13.85      A    C
ATOM   2818  C   GLY A 381       9.132  20.847  29.647  1.00 13.74      A    C
ATOM   2819  O   GLY A 381       8.096  21.259  30.153  1.00 13.57      A    O
ATOM   2820  N   ASN A 382       9.813  21.509  28.729  1.00 13.87      A    N
ATOM   2821  CA  ASN A 382       9.332  22.719  28.064  1.00 14.08      A    C
ATOM   2822  CB  ASN A 382       8.002  22.451  27.344  1.00 13.91      A    C
ATOM   2823  CG  ASN A 382       8.148  21.436  26.209  1.00 14.03      A    C
ATOM   2824  OD1 ASN A 382       9.250  21.181  25.757  1.00 13.23      A    O
ATOM   2825  ND2 ASN A 382       7.041  20.850  25.770  1.00 10.67      A    N
ATOM   2826  C   ASN A 382       9.232  23.942  28.966  1.00 14.58      A    C
ATOM   2827  O   ASN A 382       8.682  24.981  28.556  1.00 14.15      A    O
ATOM   2828  N   ASP A 383       9.796  23.869  30.178  1.00 14.75      A    N
ATOM   2829  CA  ASP A 383       9.813  25.057  31.017  1.00 14.97      A    C
ATOM   2830  CB  ASP A 383       9.593  24.709  32.499  1.00 15.34      A    C
ATOM   2831  CG  ASP A 383       9.580  25.952  33.388  1.00 15.81      A    C
ATOM   2832  OD1 ASP A 383       9.786  27.082  32.845  1.00 16.83      A    O
ATOM   2833  OD2 ASP A 383       9.394  25.897  34.636  1.00 15.84      A    O
ATOM   2834  C   ASP A 383      11.127  25.813  30.810  1.00 15.13      A    C
ATOM   2835  O   ASP A 383      12.160  25.490  31.398  1.00 15.46      A    O
ATOM   2836  N   PHE A 384      11.074  26.859  30.000  1.00 15.11      A    N
ATOM   2837  CA  PHE A 384      12.284  27.559  29.589  1.00 15.10      A    C
ATOM   2838  CB  PHE A 384      12.178  27.818  28.086  1.00 16.52      A    C
ATOM   2839  CG  PHE A 384      12.247  26.560  27.240  1.00 14.23      A    C
ATOM   2840  CD1 PHE A 384      13.440  25.910  27.059  1.00 19.41      A    C
ATOM   2841  CE1 PHE A 384      13.516  24.782  26.273  1.00 19.08      A    C
ATOM   2842  CZ  PHE A 384      12.395  24.303  25.685  1.00 18.05      A    C
ATOM   2843  CE2 PHE A 384      11.208  24.943  25.845  1.00 14.73      A    C
ATOM   2844  CD2 PHE A 384      11.140  26.070  26.602  1.00 16.74      A    C
ATOM   2845  C   PHE A 384      12.546  28.857  30.389  1.00 15.96      A    C
ATOM   2846  O   PHE A 384      13.547  29.558  30.152  1.00 15.13      A    O
ATOM   2847  N   THR A 385      11.666  29.151  31.350  1.00 16.18      A    N
ATOM   2848  CA  THR A 385      11.820  30.294  32.264  1.00 17.37      A    C
ATOM   2849  CB  THR A 385      10.519  31.097  32.400  1.00 17.19      A    C
ATOM   2850  OG1 THR A 385       9.520  30.295  33.030  1.00 17.98      A    O
ATOM   2851  CG2 THR A 385       9.922  31.491  31.028  1.00 18.21      A    C
ATOM   2852  C   THR A 385      12.238  29.868  33.689  1.00 17.95      A    C
ATOM   2853  O   THR A 385      11.703  28.890  34.252  1.00 17.41      A    O
ATOM   2854  N   ALA A 386      13.197  30.599  34.250  1.00 18.54      A    N
ATOM   2855  CA  ALA A 386      13.743  30.266  35.565  1.00 19.43      A    C
ATOM   2856  CB  ALA A 386      15.056  30.971  35.792  1.00 19.87      A    C
ATOM   2857  C   ALA A 386      12.728  30.697  36.594  1.00 20.06      A    C
ATOM   2858  O   ALA A 386      12.078  31.735  36.409  1.00 21.03      A    O
ATOM   2859  N   PRO A 387      12.525  29.897  37.635  1.00 19.71      A    N
ATOM   2860  CA  PRO A 387      13.134  28.582  37.766  1.00 20.17      A    C
ATOM   2861  CB  PRO A 387      12.951  28.269  39.250  1.00 20.90      A    C
ATOM   2862  CG  PRO A 387      11.609  28.910  39.587  1.00 20.16      A    C
ATOM   2863  CD  PRO A 387      11.670  30.223  38.796  1.00 21.11      A    C
ATOM   2864  C   PRO A 387      12.413  27.549  36.890  1.00 19.33      A    C
ATOM   2865  O   PRO A 387      11.237  27.688  36.612  1.00 18.07      A    O
ATOM   2866  N   TYR A 388      13.144  26.521  36.491  1.00 19.24      A    N
ATOM   2867  CA  TYR A 388      12.781  25.672  35.365  1.00 19.24      A    C
ATOM   2868  CB  TYR A 388      14.059  25.211  34.661  1.00 18.91      A    C
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ATOM   2869  CG  TYR A 388      14.912  26.363  34.177  1.00 18.51      A    C
ATOM   2870  CD1 TYR A 388      16.128  26.625  34.761  1.00 16.61      A    C
ATOM   2871  CE1 TYR A 388      16.912  27.701  34.350  1.00 17.76      A    C
ATOM   2872  CZ  TYR A 388      16.462  28.511  33.312  1.00 15.12      A    C
ATOM   2873  OH  TYR A 388      17.242  29.565  32.918  1.00 17.69      A    O
ATOM   2874  CE2 TYR A 388      15.241  28.276  32.723  1.00 14.50      A    C
ATOM   2875  CD2 TYR A 388      14.462  27.229  33.154  1.00 14.33      A    C
ATOM   2876  C   TYR A 388      11.934  24.467  35.745  1.00 19.73      A    C
ATOM   2877  O   TYR A 388      11.688  23.598  34.913  1.00 19.79      A    O
ATOM   2878  N   ASP A 389      11.422  24.442  36.972  1.00 20.38      A    N
ATOM   2879  CA  ASP A 389      10.605  23.327  37.430  1.00 21.41      A    C
ATOM   2880  CB  ASP A 389      11.346  22.547  38.507  1.00 22.04      A    C
ATOM   2881  CG  ASP A 389      11.504  23.343  39.796  1.00 24.83      A    C
ATOM   2882  OD1 ASP A 389      11.618  22.706  40.869  1.00 27.95      A    O
ATOM   2883  OD2 ASP A 389      11.523  24.595  39.822  1.00 24.63      A    O
ATOM   2884  C   ASP A 389       9.246  23.724  37.968  1.00 21.64      A    C
ATOM   2885  O   ASP A 389       8.629  22.947  38.709  1.00 22.12      A    O
ATOM   2886  N   ASN A 390       8.759  24.908  37.618  1.00 21.45      A    N
ATOM   2887  CA  ASN A 390       7.455  25.326  38.130  1.00 22.14      A    C
ATOM   2888  CB  ASN A 390       7.555  26.664  38.892  1.00 22.91      A    C
ATOM   2889  CG  ASN A 390       7.965  27.825  37.989  1.00 23.08      A    C
ATOM   2890  OD1 ASN A 390       8.404  27.620  36.847  1.00 22.98      A    O
ATOM   2891  ND2 ASN A 390       7.816  29.050  38.491  1.00 23.21      A    N
ATOM   2892  C   ASN A 390       6.356  25.402  37.060  1.00 22.16      A    C
ATOM   2893  O   ASN A 390       5.181  25.500  37.405  1.00 21.88      A    O
ATOM   2894  N   ASN A 391       6.717  25.340  35.772  1.00 21.51      A    N
ATOM   2895  CA  ASN A 391       5.705  25.411  34.713  1.00 20.98      A    C
ATOM   2896  CB  ASN A 391       5.986  26.567  33.728  1.00 21.22      A    C
ATOM   2897  CG  ASN A 391       6.221  27.924  34.426  1.00 22.34      A    C
ATOM   2898  OD1 ASN A 391       7.345  28.481  34.388  1.00 22.21      A    O
ATOM   2899  ND2 ASN A 391       5.151  28.490  35.029  1.00 23.08      A    N
ATOM   2900  C   ASN A 391       5.611  24.072  33.978  1.00 20.79      A    C
ATOM   2901  O   ASN A 391       6.295  23.818  32.978  1.00 21.08      A    O
ATOM   2902  N   TRP A 392       4.741  23.211  34.467  1.00 20.10      A    N
ATOM   2903  CA  TRP A 392       4.601  21.862  33.928  1.00 20.04      A    C
ATOM   2904  CB  TRP A 392       3.893  20.979  34.926  1.00 20.74      A    C
ATOM   2905  CG  TRP A 392       4.629  20.757  36.231  1.00 24.30      A    C
ATOM   2906  CD1 TRP A 392       4.687  21.605  37.309  1.00 28.54      A    C
ATOM   2907  NE1 TRP A 392       5.435  21.038  38.317  1.00 30.71      A    N
ATOM   2908  CE2 TRP A 392       5.870  19.804  37.902  1.00 28.29      A    C
ATOM   2909  CD2 TRP A 392       5.367  19.594  36.598  1.00 27.17      A    C
ATOM   2910  CE3 TRP A 392       5.695  18.400  35.937  1.00 29.38      A    C
ATOM   2911  CZ3 TRP A 392       6.456  17.447  36.608  1.00 28.54      A    C
ATOM   2912  CH2 TRP A 392       6.922  17.683  37.904  1.00 30.49      A    C
ATOM   2913  CZ2 TRP A 392       6.643  18.857  38.566  1.00 30.31      A    C
ATOM   2914  C   TRP A 392       3.767  21.890  32.661  1.00 19.03      A    C
ATOM   2915  O   TRP A 392       2.828  22.678  32.552  1.00 19.40      A    O
ATOM   2916  N   ASP A 393       4.107  21.020  31.709  1.00 17.66      A    N
ATOM   2917  CA  ASP A 393       3.416  20.958  30.424  1.00 16.59      A    C
ATOM   2918  CB  ASP A 393       4.431  20.669  29.332  1.00 16.47      A    C
ATOM   2919  CG  ASP A 393       3.813  20.660  27.930  1.00 15.80      A    C
ATOM   2920  OD1 ASP A 393       4.350  21.364  27.045  1.00 14.98      A    O
ATOM   2921  OD2 ASP A 393       2.817  19.975  27.629  1.00 15.12      A    O
ATOM   2922  C   ASP A 393       2.324  19.888  30.425  1.00 16.46      A    C
ATOM   2923  O   ASP A 393       2.606  18.716  30.648  1.00 15.65      A    O
ATOM   2924  N   GLY A 394       1.080  20.302  30.178  1.00 15.96      A    N
ATOM   2925  CA  GLY A 394      -0.029  19.384  30.014  1.00 16.13      A    C
ATOM   2926  C   GLY A 394      -0.747  19.498  28.675  1.00 16.27      A    C
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ATOM	2927	O	GLY	A	394	-1.936	19.255	28.601	1.00	16.15	A	O
ATOM	2928	N	ARG	A	395	-0.030	19.864	27.617	1.00	17.31	A	N
ATOM	2929	CA	ARG	A	395	-0.607	19.978	26.264	1.00	17.68	A	C
ATOM	2930	CB	ARG	A	395	-0.588	21.437	25.783	1.00	19.08	A	C
ATOM	2931	CG	ARG	A	395	-1.434	22.408	26.518	1.00	26.02	A	C
ATOM	2932	CD	ARG	A	395	-1.172	23.839	26.066	1.00	31.34	A	C
ATOM	2933	NE	ARG	A	395	-1.802	24.813	26.969	1.00	37.30	A	N
ATOM	2934	CZ	ARG	A	395	-3.026	25.331	26.821	1.00	40.58	A	C
ATOM	2935	NH1	ARG	A	395	-3.478	26.216	27.717	1.00	44.12	A	N
ATOM	2936	NH2	ARG	A	395	-3.805	24.983	25.805	1.00	40.20	A	N
ATOM	2937	C	ARG	A	395	0.176	19.240	25.165	1.00	15.80	A	C
ATOM	2938	O	ARG	A	395	-0.418	18.827	24.176	1.00	16.01	A	O
ATOM	2939	N	ASN	A	396	1.502	19.212	25.282	1.00	14.41	A	N
ATOM	2940	CA	ASN	A	396	2.389	18.645	24.251	1.00	13.89	A	C
ATOM	2941	CB	ASN	A	396	3.662	19.483	24.133	1.00	13.10	A	C
ATOM	2942	CG	ASN	A	396	3.408	20.889	23.585	1.00	14.63	A	C
ATOM	2943	OD1	ASN	A	396	3.129	21.075	22.374	1.00	11.53	A	O
ATOM	2944	ND2	ASN	A	396	3.550	21.897	24.463	1.00	11.89	A	N
ATOM	2945	C	ASN	A	396	2.806	17.197	24.475	1.00	13.64	A	C
ATOM	2946	O	ASN	A	396	2.995	16.743	25.634	1.00	14.92	A	O
ATOM	2947	N	ASN	A	397	2.973	16.452	23.376	1.00	13.56	A	N
ATOM	2948	CA	ASN	A	397	3.539	15.085	23.451	1.00	12.37	A	C
ATOM	2949	CB	ASN	A	397	2.705	14.080	22.672	1.00	12.41	A	C
ATOM	2950	CG	ASN	A	397	2.539	14.450	21.192	1.00	13.07	A	C
ATOM	2951	OD1	ASN	A	397	2.243	15.594	20.849	1.00	12.07	A	O
ATOM	2952	ND2	ASN	A	397	2.683	13.466	20.324	1.00	13.08	A	N
ATOM	2953	C	ASN	A	397	5.011	15.077	23.010	1.00	13.13	A	C
ATOM	2954	O	ASN	A	397	5.607	14.010	22.663	1.00	11.34	A	O
ATOM	2955	N	VAL	A	398	5.577	16.291	23.028	1.00	12.66	A	N
ATOM	2956	CA	VAL	A	398	6.992	16.524	22.914	1.00	12.58	A	C
ATOM	2957	CB	VAL	A	398	7.329	17.261	21.626	1.00	13.06	A	C
ATOM	2958	CG1	VAL	A	398	8.835	17.523	21.533	1.00	11.41	A	C
ATOM	2959	CG2	VAL	A	398	6.846	16.476	20.408	1.00	12.98	A	C
ATOM	2960	C	VAL	A	398	7.381	17.412	24.105	1.00	12.92	A	C
ATOM	2961	O	VAL	A	398	6.819	18.501	24.272	1.00	13.08	A	O
ATOM	2962	N	GLU	A	399	8.288	16.913	24.945	1.00	12.47	A	N
ATOM	2963	CA	GLU	A	399	8.797	17.666	26.107	1.00	12.81	A	C
ATOM	2964	CB	GLU	A	399	8.339	17.054	27.452	1.00	12.40	A	C
ATOM	2965	CG	GLU	A	399	6.870	17.340	27.793	1.00	11.56	A	C
ATOM	2966	CD	GLU	A	399	6.538	17.357	29.284	1.00	13.58	A	C
ATOM	2967	OE1	GLU	A	399	5.312	17.324	29.635	1.00	14.48	A	O
ATOM	2968	OE2	GLU	A	399	7.471	17.421	30.112	1.00	14.20	A	O
ATOM	2969	C	GLU	A	399	10.307	17.680	26.052	1.00	12.44	A	C
ATOM	2970	O	GLU	A	399	10.920	16.624	25.929	1.00	13.16	A	O
ATOM	2971	N	ASN	A	400	10.890	18.883	26.174	1.00	12.69	A	N
ATOM	2972	CA	ASN	A	400	12.326	19.098	26.073	1.00	12.36	A	C
ATOM	2973	CB	ASN	A	400	12.636	19.953	24.822	1.00	12.37	A	C
ATOM	2974	CG	ASN	A	400	12.185	19.302	23.559	1.00	14.26	A	C
ATOM	2975	OD1	ASN	A	400	12.621	18.213	23.247	1.00	16.94	A	O
ATOM	2976	ND2	ASN	A	400	11.302	19.964	22.817	1.00	14.56	A	N
ATOM	2977	C	ASN	A	400	12.959	19.820	27.254	1.00	11.55	A	C
ATOM	2978	O	ASN	A	400	12.363	20.716	27.867	1.00	11.03	A	O
ATOM	2979	N	VAL	A	401	14.200	19.448	27.543	1.00	11.83	A	N
ATOM	2980	CA	VAL	A	401	15.042	20.183	28.494	1.00	11.67	A	C
ATOM	2981	CB	VAL	A	401	15.230	19.394	29.804	1.00	11.24	A	C
ATOM	2982	CG1	VAL	A	401	16.317	20.017	30.668	1.00	13.18	A	C
ATOM	2983	CG2	VAL	A	401	13.962	19.359	30.558	1.00	11.36	A	C
ATOM	2984	C	VAL	A	401	16.351	20.372	27.792	1.00	12.10	A	C

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ATOM   2985  O   VAL A 401      17.022  19.394  27.471  1.00 12.05      A    O
ATOM   2986  N   PHE A 402      16.693  21.634  27.528  1.00 12.69      A    N
ATOM   2987  CA  PHE A 402      17.841  22.019  26.744  1.00 14.06      A    C
ATOM   2988  CB  PHE A 402      17.401  22.853  25.517  1.00 14.70      A    C
ATOM   2989  CG  PHE A 402      16.602  22.079  24.464  1.00 12.42      A    C
ATOM   2990  CD1 PHE A 402      15.936  22.764  23.455  1.00 15.18      A    C
ATOM   2991  CE1 PHE A 402      15.222  22.069  22.468  1.00 12.37      A    C
ATOM   2992  CZ  PHE A 402      15.195  20.700  22.489  1.00 11.68      A    C
ATOM   2993  CE2 PHE A 402      15.841  20.022  23.493  1.00 14.06      A    C
ATOM   2994  CD2 PHE A 402      16.534  20.698  24.465  1.00 10.95      A    C
ATOM   2995  C   PHE A 402      18.725  22.896  27.641  1.00 15.85      A    C
ATOM   2996  O   PHE A 402      18.356  24.021  27.952  1.00 16.80      A    O
ATOM   2997  N   ILE A 403      19.886  22.379  28.028  1.00 16.60      A    N
ATOM   2998  CA  ILE A 403      20.787  23.062  28.963  1.00 17.41      A    C
ATOM   2999  CB  ILE A 403      21.088  22.167  30.160  1.00 16.74      A    C
ATOM   3000  CG1 ILE A 403      19.802  21.886  30.944  1.00 17.16      A    C
ATOM   3001  CD1 ILE A 403      19.946  20.733  31.931  1.00 15.43      A    C
ATOM   3002  CG2 ILE A 403      22.143  22.809  31.095  1.00 17.20      A    C
ATOM   3003  C   ILE A 403      22.064  23.395  28.240  1.00 17.62      A    C
ATOM   3004  O   ILE A 403      22.812  22.520  27.854  1.00 17.97      A    O
ATOM   3005  N   ASN A 404      22.299  24.678  28.026  1.00 18.39      A    N
ATOM   3006  CA  ASN A 404      23.429  25.112  27.231  1.00 19.61      A    C
ATOM   3007  CB  ASN A 404      23.255  26.599  26.874  1.00 20.94      A    C
ATOM   3008  CG  ASN A 404      24.297  27.071  25.913  1.00 26.59      A    C
ATOM   3009  OD1 ASN A 404      24.339  26.618  24.752  1.00 32.24      A    O
ATOM   3010  ND2 ASN A 404      25.177  27.980  26.381  1.00 32.91      A    N
ATOM   3011  C   ASN A 404      24.773  24.892  27.940  1.00 18.94      A    C
ATOM   3012  O   ASN A 404      25.769  24.575  27.296  1.00 18.69      A    O
ATOM   3013  N   ALA A 405      24.779  25.020  29.262  1.00 18.60      A    N
ATOM   3014  CA  ALA A 405      26.011  24.902  30.044  1.00 19.42      A    C
ATOM   3015  CB  ALA A 405      26.450  26.317  30.582  1.00 19.40      A    C
ATOM   3016  C   ALA A 405      25.787  23.934  31.217  1.00 19.12      A    C
ATOM   3017  O   ALA A 405      25.582  24.364  32.360  1.00 18.74      A    O
ATOM   3018  N   PRO A 406      25.782  22.632  30.936  1.00 19.16      A    N
ATOM   3019  CA  PRO A 406      25.508  21.629  31.977  1.00 19.37      A    C
ATOM   3020  CB  PRO A 406      25.266  20.351  31.156  1.00 19.25      A    C
ATOM   3021  CG  PRO A 406      26.120  20.546  29.977  1.00 19.80      A    C
ATOM   3022  CD  PRO A 406      26.033  22.010  29.631  1.00 18.90      A    C
ATOM   3023  C   PRO A 406      26.689  21.437  32.923  1.00 19.45      A    C
ATOM   3024  O   PRO A 406      27.815  21.833  32.607  1.00 19.95      A    O
ATOM   3025  N   GLN A 407      26.437  20.819  34.072  1.00 19.97      A    N
ATOM   3026  CA  GLN A 407      27.490  20.446  35.016  1.00 20.20      A    C
ATOM   3027  CB  GLN A 407      26.908  20.387  36.413  1.00 21.02      A    C
ATOM   3028  CG  GLN A 407      26.155  21.620  36.805  1.00 22.32      A    C
ATOM   3029  CD  GLN A 407      25.122  21.323  37.849  1.00 23.76      A    C
ATOM   3030  OE1 GLN A 407      25.320  20.443  38.713  1.00 21.20      A    O
ATOM   3031  NE2 GLN A 407      24.016  22.040  37.789  1.00 22.99      A    N
ATOM   3032  C   GLN A 407      28.062  19.075  34.675  1.00 20.27      A    C
ATOM   3033  O   GLN A 407      27.392  18.232  34.057  1.00 19.75      A    O
ATOM   3034  N   SER A 408      29.294  18.830  35.099  1.00 20.30      A    N
ATOM   3035  CA  SER A 408      29.869  17.491  35.033  1.00 20.08      A    C
ATOM   3036  CB  SER A 408      31.393  17.538  35.212  1.00 20.55      A    C
ATOM   3037  OG  SER A 408      32.042  18.067  34.072  1.00 19.34      A    O
ATOM   3038  C   SER A 408      29.269  16.615  36.120  1.00 19.97      A    C
ATOM   3039  O   SER A 408      29.130  17.043  37.268  1.00 20.96      A    O
ATOM   3040  N   GLY A 409      28.980  15.362  35.775  1.00 19.80      A    N
ATOM   3041  CA  GLY A 409      28.447  14.392  36.715  1.00 18.94      A    C
ATOM   3042  C   GLY A 409      27.216  13.697  36.160  1.00 19.28      A    C
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ATOM   3043  O   GLY A 409      27.026  13.646  34.940  1.00 18.32      A    O
ATOM   3044  N   THR A 410      26.350  13.224  37.058  1.00 18.72      A    N
ATOM   3045  CA  THR A 410      25.226  12.396  36.678  1.00 18.26      A    C
ATOM   3046  CB  THR A 410      25.105  11.220  37.631  1.00 17.98      A    C
ATOM   3047  OG1 THR A 410      26.334  10.466  37.637  1.00 16.34      A    O
ATOM   3048  CG2 THR A 410      24.038  10.227  37.136  1.00 18.99      A    C
ATOM   3049  C   THR A 410      23.923  13.183  36.687  1.00 18.19      A    C
ATOM   3050  O   THR A 410      23.510  13.735  37.718  1.00 18.85      A    O
ATOM   3051  N   TYR A 411      23.274  13.241  35.524  1.00 17.34      A    N
ATOM   3052  CA  TYR A 411      21.942  13.783  35.430  1.00 16.46      A    C
ATOM   3053  CB  TYR A 411      21.731  14.459  34.067  1.00 16.84      A    C
ATOM   3054  CG  TYR A 411      22.286  15.869  34.025  1.00 16.33      A    C
ATOM   3055  CD1 TYR A 411      21.458  16.953  34.156  1.00 16.27      A    C
ATOM   3056  CE1 TYR A 411      21.956  18.231  34.131  1.00 16.41      A    C
ATOM   3057  CZ  TYR A 411      23.319  18.438  33.994  1.00 17.03      A    C
ATOM   3058  OH  TYR A 411      23.789  19.744  34.031  1.00 17.03      A    O
ATOM   3059  CE2 TYR A 411      24.172  17.380  33.880  1.00 16.15      A    C
ATOM   3060  CD2 TYR A 411      23.660  16.099  33.889  1.00 17.36      A    C
ATOM   3061  C   TYR A 411      20.956  12.627  35.606  1.00 16.14      A    C
ATOM   3062  O   TYR A 411      21.157  11.557  35.041  1.00 15.95      A    O
ATOM   3063  N   THR A 412      19.920  12.841  36.399  1.00 15.50      A    N
ATOM   3064  CA  THR A 412      18.760  11.959  36.418  1.00 16.39      A    C
ATOM   3065  CB  THR A 412      18.107  12.037  37.808  1.00 16.73      A    C
ATOM   3066  OG1 THR A 412      19.041  11.544  38.783  1.00 16.43      A    O
ATOM   3067  CG2 THR A 412      16.877  11.115  37.946  1.00 18.16      A    C
ATOM   3068  C   THR A 412      17.764  12.397  35.344  1.00 16.26      A    C
ATOM   3069  O   THR A 412      17.404  13.568  35.286  1.00 15.84      A    O
ATOM   3070  N   VAL A 413      17.313  11.444  34.516  1.00 16.67      A    N
ATOM   3071  CA  VAL A 413      16.342  11.672  33.452  1.00 15.75      A    C
ATOM   3072  CB  VAL A 413      16.924  11.246  32.066  1.00 16.41      A    C
ATOM   3073  CG1 VAL A 413      15.914  11.476  30.914  1.00 15.53      A    C
ATOM   3074  CG2 VAL A 413      18.240  11.946  31.773  1.00 15.42      A    C
ATOM   3075  C   VAL A 413      15.134  10.811  33.791  1.00 16.95      A    C
ATOM   3076  O   VAL A 413      15.232   9.574  33.667  1.00 18.21      A    O
ATOM   3077  N   GLU A 414      14.040  11.439  34.256  1.00 16.21      A    N
ATOM   3078  CA  GLU A 414      12.803  10.774  34.736  1.00 17.01      A    C
ATOM   3079  CB  GLU A 414      12.467  11.202  36.134  1.00 16.06      A    C
ATOM   3080  CG  GLU A 414      11.518  10.244  36.767  1.00 18.61      A    C
ATOM   3081  CD  GLU A 414      11.626  10.318  38.265  1.00 17.99      A    C
ATOM   3082  OE1 GLU A 414      11.212  11.334  38.830  1.00 20.38      A    O
ATOM   3083  OE2 GLU A 414      12.198   9.404  38.810  1.00 18.55      A    O
ATOM   3084  C   GLU A 414      11.715  11.142  33.729  1.00 16.05      A    C
ATOM   3085  O   GLU A 414      11.428  12.301  33.528  1.00 15.27      A    O
ATOM   3086  N   VAL A 415      11.037  10.172  33.145  1.00 16.93      A    N
ATOM   3087  CA  VAL A 415       9.622  10.184  32.847  1.00 16.73      A    C
ATOM   3088  CB  VAL A 415       9.472   9.367  31.526  1.00 17.17      A    C
ATOM   3089  CG1 VAL A 415       8.168   9.660  30.813  1.00 16.00      A    C
ATOM   3090  CG2 VAL A 415      10.652   9.660  30.622  1.00 16.72      A    C
ATOM   3091  C   VAL A 415       8.540   9.769  33.787  1.00 16.71      A    C
ATOM   3092  O   VAL A 415       8.463   8.634  34.185  1.00 16.19      A    O
ATOM   3093  N   GLN A 416       7.684  10.736  34.077  1.00 16.05      A    N
ATOM   3094  CA  GLN A 416       6.553  10.579  34.989  1.00 16.43      A    C
ATOM   3095  CB  GLN A 416       6.519  11.747  35.981  1.00 16.01      A    C
ATOM   3096  CG  GLN A 416       7.786  11.832  36.802  1.00 16.27      A    C
ATOM   3097  CD  GLN A 416       7.821  12.929  37.827  1.00 17.22      A    C
ATOM   3098  OE1 GLN A 416       6.912  13.762  37.905  1.00 16.47      A    O
ATOM   3099  NE2 GLN A 416       8.933  12.972  38.601  1.00 16.72      A    N
ATOM   3100  C   GLN A 416       5.232  10.504  34.235  1.00 17.01      A    C
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ATOM   3101  O   GLN A 416       4.899  11.388  33.440  1.00 16.94      A    O
ATOM   3102  N   ALA A 417       4.461   9.462  34.522  1.00 17.66      A    N
ATOM   3103  CA  ALA A 417       3.122   9.307  33.953  1.00 18.17      A    C
ATOM   3104  CB  ALA A 417       2.770   7.857  33.891  1.00 18.16      A    C
ATOM   3105  C   ALA A 417       2.092  10.083  34.790  1.00 19.19      A    C
ATOM   3106  O   ALA A 417       1.542   9.565  35.775  1.00 18.61      A    O
ATOM   3107  N   TYR A 418       1.859  11.338  34.437  1.00 19.27      A    N
ATOM   3108  CA  TYR A 418       0.944  12.153  35.234  1.00 20.10      A    C
ATOM   3109  CB  TYR A 418       0.985  13.618  34.803  1.00 20.65      A    C
ATOM   3110  CG  TYR A 418       0.021  14.496  35.570  1.00 23.36      A    C
ATOM   3111  CD1 TYR A 418       0.255  14.818  36.908  1.00 26.20      A    C
ATOM   3112  CE1 TYR A 418      -0.645  15.610  37.625  1.00 29.96      A    C
ATOM   3113  CZ  TYR A 418      -1.772  16.099  36.990  1.00 31.45      A    C
ATOM   3114  OH  TYR A 418      -2.659  16.888  37.685  1.00 34.45      A    O
ATOM   3115  CE2 TYR A 418      -2.018  15.804  35.652  1.00 29.32      A    C
ATOM   3116  CD2 TYR A 418      -1.123  15.002  34.957  1.00 26.35      A    C
ATOM   3117  C   TYR A 418      -0.477  11.623  35.158  1.00 19.95      A    C
ATOM   3118  O   TYR A 418      -1.142  11.445  36.190  1.00 19.83      A    O
ATOM   3119  N   ASN A 419      -0.928  11.332  33.945  1.00 19.39      A    N
ATOM   3120  CA  ASN A 419      -2.284  10.855  33.708  1.00 19.40      A    C
ATOM   3121  CB  ASN A 419      -3.243  12.051  33.629  1.00 20.03      A    C
ATOM   3122  CG  ASN A 419      -4.705  11.625  33.611  1.00 21.53      A    C
ATOM   3123  OD1 ASN A 419      -5.094  10.758  34.354  1.00 23.42      A    O
ATOM   3124  ND2 ASN A 419      -5.493  12.212  32.727  1.00 22.67      A    N
ATOM   3125  C   ASN A 419      -2.374  10.079  32.402  1.00 19.75      A    C
ATOM   3126  O   ASN A 419      -2.186  10.646  31.317  1.00 19.24      A    O
ATOM   3127  N   VAL A 420      -2.703   8.795  32.486  1.00 19.24      A    N
ATOM   3128  CA  VAL A 420      -2.744   7.948  31.295  1.00 18.57      A    C
ATOM   3129  CB  VAL A 420      -1.533   6.986  31.288  1.00 18.55      A    C
ATOM   3130  CG1 VAL A 420      -1.504   6.086  30.040  1.00 17.15      A    C
ATOM   3131  CG2 VAL A 420      -0.196   7.799  31.402  1.00 20.43      A    C
ATOM   3132  C   VAL A 420      -4.067   7.165  31.234  1.00 18.55      A    C
ATOM   3133  O   VAL A 420      -4.109   5.996  31.606  1.00 18.55      A    O
ATOM   3134  N   PRO A 421      -5.132   7.816  30.776  1.00 18.79      A    N
ATOM   3135  CA  PRO A 421      -6.444   7.169  30.635  1.00 19.54      A    C
ATOM   3136  CB  PRO A 421      -7.397   8.324  30.288  1.00 19.65      A    C
ATOM   3137  CG  PRO A 421      -6.540   9.394  29.746  1.00 19.70      A    C
ATOM   3138  CD  PRO A 421      -5.175   9.239  30.396  1.00 18.68      A    C
ATOM   3139  C   PRO A 421      -6.507   6.141  29.530  1.00 19.68      A    C
ATOM   3140  O   PRO A 421      -7.411   5.318  29.565  1.00 20.15      A    O
ATOM   3141  N   VAL A 422      -5.592   6.178  28.566  1.00 19.04      A    N
ATOM   3142  CA  VAL A 422      -5.594   5.180  27.505  1.00 18.85      A    C
ATOM   3143  CB  VAL A 422      -5.990   5.781  26.146  1.00 18.35      A    C
ATOM   3144  CG1 VAL A 422      -6.200   4.653  25.091  1.00 18.91      A    C
ATOM   3145  CG2 VAL A 422      -7.264   6.616  26.285  1.00 18.28      A    C
ATOM   3146  C   VAL A 422      -4.226   4.509  27.448  1.00 19.38      A    C
ATOM   3147  O   VAL A 422      -3.435   4.713  26.505  1.00 18.38      A    O
ATOM   3148  N   GLY A 423      -3.957   3.707  28.480  1.00 19.46      A    N
ATOM   3149  CA  GLY A 423      -2.642   3.150  28.702  1.00 19.62      A    C
ATOM   3150  C   GLY A 423      -2.510   1.665  28.496  1.00 19.72      A    C
ATOM   3151  O   GLY A 423      -3.464   0.954  28.162  1.00 21.71      A    O
ATOM   3152  N   PRO A 424      -1.307   1.174  28.695  1.00 19.10      A    N
ATOM   3153  CA  PRO A 424      -0.142   1.999  29.040  1.00 17.55      A    C
ATOM   3154  CB  PRO A 424       0.876   0.969  29.467  1.00 18.01      A    C
ATOM   3155  CG  PRO A 424       0.510  -0.258  28.696  1.00 19.87      A    C
ATOM   3156  CD  PRO A 424      -0.988  -0.267  28.649  1.00 19.26      A    C
ATOM   3157  C   PRO A 424       0.396   2.842  27.899  1.00 16.87      A    C
ATOM   3158  O   PRO A 424       0.038   2.660  26.733  1.00 17.20      A    O
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ATOM   3159  N   GLN A 425      1.248   3.798  28.239  1.00 15.38      A    N
ATOM   3160  CA  GLN A 425      1.848   4.678  27.240  1.00 14.36      A    C
ATOM   3161  CB  GLN A 425      1.507   6.140  27.559  1.00 14.88      A    C
ATOM   3162  CG  GLN A 425      2.070   7.202  26.576  1.00 14.70      A    C
ATOM   3163  CD  GLN A 425      1.512   7.043  25.180  1.00 16.71      A    C
ATOM   3164  OE1 GLN A 425      0.321   7.321  24.956  1.00 15.27      A    O
ATOM   3165  NE2 GLN A 425      2.349   6.580  24.235  1.00 11.93      A    N
ATOM   3166  C   GLN A 425      3.341   4.470  27.252  1.00 13.10      A    C
ATOM   3167  O   GLN A 425      3.987   4.662  28.283  1.00 12.18      A    O
ATOM   3168  N   THR A 426      3.887   4.036  26.112  1.00 12.88      A    N
ATOM   3169  CA  THR A 426      5.320   4.008  25.913  1.00 12.90      A    C
ATOM   3170  CB  THR A 426      5.737   2.949  24.890  1.00 12.37      A    C
ATOM   3171  OG1 THR A 426      5.134   3.254  23.626  1.00 12.70      A    O
ATOM   3172  CG2 THR A 426      5.232   1.573  25.283  1.00 13.56      A    C
ATOM   3173  C   THR A 426      5.796   5.370  25.413  1.00 13.16      A    C
ATOM   3174  O   THR A 426      4.986   6.223  25.037  1.00 14.38      A    O
ATOM   3175  N   PHE A 427      7.115   5.551  25.401  1.00 12.86      A    N
ATOM   3176  CA  PHE A 427      7.741   6.823  25.036  1.00 12.44      A    C
ATOM   3177  CB  PHE A 427      7.802   7.778  26.240  1.00 12.42      A    C
ATOM   3178  CG  PHE A 427      8.612   7.235  27.366  1.00 12.82      A    C
ATOM   3179  CD1 PHE A 427      9.988   7.361  27.365  1.00 15.21      A    C
ATOM   3180  CE1 PHE A 427     10.768   6.801  28.381  1.00 15.74      A    C
ATOM   3181  CZ  PHE A 427     10.161   6.102  29.408  1.00 14.88      A    C
ATOM   3182  CE2 PHE A 427      8.766   5.987  29.427  1.00 16.39      A    C
ATOM   3183  CD2 PHE A 427      8.000   6.538  28.407  1.00 14.33      A    C
ATOM   3184  C   PHE A 427      9.149   6.532  24.549  1.00 12.14      A    C
ATOM   3185  O   PHE A 427      9.694   5.444  24.807  1.00 11.55      A    O
ATOM   3186  N   SER A 428      9.721   7.523  23.867  1.00 11.59      A    N
ATOM   3187  CA  SER A 428     11.116   7.528  23.480  1.00 11.99      A    C
ATOM   3188  CB  SER A 428     11.292   7.463  21.965  1.00 12.17      A    C
ATOM   3189  OG  SER A 428     10.837   6.219  21.442  1.00 12.32      A    O
ATOM   3190  C   SER A 428     11.804   8.776  24.031  1.00 12.57      A    C
ATOM   3191  O   SER A 428     11.174   9.829  24.263  1.00 11.91      A    O
ATOM   3192  N   LEU A 429     13.103   8.620  24.278  1.00 12.35      A    N
ATOM   3193  CA  LEU A 429     13.950   9.712  24.714  1.00 12.57      A    C
ATOM   3194  CB  LEU A 429     14.508   9.476  26.135  1.00 12.84      A    C
ATOM   3195  CG  LEU A 429     13.542   9.648  27.296  1.00 13.77      A    C
ATOM   3196  CD1 LEU A 429     14.046   8.907  28.520  1.00 15.69      A    C
ATOM   3197  CD2 LEU A 429     13.348  11.110  27.609  1.00 15.64      A    C
ATOM   3198  C   LEU A 429     15.098   9.756  23.768  1.00 11.82      A    C
ATOM   3199  O   LEU A 429     15.593   8.707  23.372  1.00 11.44      A    O
ATOM   3200  N   ALA A 430     15.532  10.957  23.405  1.00 11.55      A    N
ATOM   3201  CA  ALA A 430     16.805  11.139  22.699  1.00 11.87      A    C
ATOM   3202  CB  ALA A 430     16.581  11.528  21.235  1.00 12.63      A    C
ATOM   3203  C   ALA A 430     17.613  12.215  23.404  1.00 12.76      A    C
ATOM   3204  O   ALA A 430     17.072  13.256  23.776  1.00 12.14      A    O
ATOM   3205  N   ILE A 431     18.907  11.943  23.584  1.00 12.52      A    N
ATOM   3206  CA  ILE A 431     19.813  12.835  24.287  1.00 13.32      A    C
ATOM   3207  CB  ILE A 431     20.325  12.179  25.593  1.00 13.00      A    C
ATOM   3208  CG1 ILE A 431     19.175  11.882  26.542  1.00 14.30      A    C
ATOM   3209  CD1 ILE A 431     19.575  11.061  27.776  1.00 16.21      A    C
ATOM   3210  CG2 ILE A 431     21.292  13.123  26.288  1.00 14.86      A    C
ATOM   3211  C   ILE A 431     21.005  13.176  23.392  1.00 12.92      A    C
ATOM   3212  O   ILE A 431     21.728  12.288  22.937  1.00 11.26      A    O
ATOM   3213  N   VAL A 432     21.192  14.464  23.134  1.00 13.80      A    N
ATOM   3214  CA  VAL A 432     22.387  14.966  22.483  1.00 15.20      A    C
ATOM   3215  CB  VAL A 432     22.028  15.996  21.387  1.00 15.89      A    C
ATOM   3216  CG1 VAL A 432     23.293  16.591  20.809  1.00 15.25      A    C
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ATOM   3217  CG2 VAL A 432      21.167  15.361  20.293  1.00 15.39      A    C
ATOM   3218  C   VAL A 432      23.346  15.634  23.498  1.00 16.38      A    C
ATOM   3219  O   VAL A 432      22.923  16.472  24.298  1.00 16.49      A    O
ATOM   3220  N   HIS A 433      24.633  15.257  23.458  1.00 17.45      A    N
ATOM   3221  CA  HIS A 433      25.669  15.872  24.306  1.00 18.55      A    C
ATOM   3222  CB  HIS A 433      25.637  15.240  25.711  1.00 19.21      A    C
ATOM   3223  CG  HIS A 433      26.553  15.885  26.707  1.00 19.32      A    C
ATOM   3224  ND1 HIS A 433      26.497  17.233  27.015  1.00 18.22      A    N
ATOM   3225  CE1 HIS A 433      27.378  17.497  27.969  1.00 18.90      A    C
ATOM   3226  NE2 HIS A 433      27.999  16.380  28.289  1.00 16.51      A    N
ATOM   3227  CD2 HIS A 433      27.502  15.353  27.513  1.00 17.65      A    C
ATOM   3228  C   HIS A 433      27.031  15.627  23.684  1.00 19.74      A    C
ATOM   3229  O   HIS A 433      27.664  16.546  23.133  1.00 21.68      A    O
ATOM   3230  OXT HIS A 433      27.463  14.480  23.735  1.00 19.29      A    O
TER    3230      HIS A 433
HETATM 3231  CA  CA  A 601      15.429  35.876   3.369  1.00 16.92      A   CA
HETATM 3232  CA  CA  A 602       3.346  16.597  30.346  1.00 13.45      A   CA
HETATM 3233  CA  CA  A 603       9.615  28.353  34.891  1.00 17.30      A   CA
ATOM   3234  N   ASP B  16       3.955  53.303 -10.201  1.00 49.01      B    N
ATOM   3235  CA  ASP B  16       4.171  51.870  -9.771  1.00 49.32      B    C
ATOM   3236  CB  ASP B  16       5.553  51.425 -10.270  1.00 49.78      B    C
ATOM   3237  CG  ASP B  16       6.176  52.438 -11.248  1.00 52.12      B    C
ATOM   3238  OD1 ASP B  16       5.667  52.549 -12.399  1.00 54.86      B    O
ATOM   3239  OD2 ASP B  16       7.151  53.181 -10.957  1.00 52.51      B    O
ATOM   3240  C   ASP B  16       4.009  51.690  -8.232  1.00 48.45      B    C
ATOM   3241  O   ASP B  16       4.793  50.996  -7.567  1.00 47.87      B    O
ATOM   3242  N   ARG B  17       2.959  52.301  -7.687  1.00 47.87      B    N
ATOM   3243  CA  ARG B  17       2.863  52.592  -6.247  1.00 47.30      B    C
ATOM   3244  CB  ARG B  17       2.430  54.064  -6.059  1.00 46.77      B    C
ATOM   3245  CG  ARG B  17       3.107  55.055  -7.028  1.00 44.50      B    C
ATOM   3246  CD  ARG B  17       2.860  56.528  -6.691  1.00 39.98      B    C
ATOM   3247  NE  ARG B  17       3.266  56.891  -5.335  1.00 33.05      B    N
ATOM   3248  CZ  ARG B  17       4.483  57.334  -5.001  1.00 29.36      B    C
ATOM   3249  NH1 ARG B  17       5.440  57.459  -5.915  1.00 28.07      B    N
ATOM   3250  NH2 ARG B  17       4.752  57.650  -3.740  1.00 24.57      B    N
ATOM   3251  C   ARG B  17       1.917  51.699  -5.415  1.00 48.01      B    C
ATOM   3252  O   ARG B  17       1.463  52.120  -4.342  1.00 47.42      B    O
ATOM   3253  N   HIS B  18       1.616  50.486  -5.885  1.00 48.51      B    N
ATOM   3254  CA  HIS B  18       0.770  49.573  -5.108  1.00 48.98      B    C
ATOM   3255  CB  HIS B  18       0.515  48.266  -5.875  1.00 49.29      B    C
ATOM   3256  CG  HIS B  18      -0.510  48.388  -6.961  1.00 50.05      B    C
ATOM   3257  ND1 HIS B  18      -0.195  48.803  -8.238  1.00 51.24      B    N
ATOM   3258  CE1 HIS B  18      -1.291  48.814  -8.979  1.00 51.27      B    C
ATOM   3259  NE2 HIS B  18      -2.305  48.419  -8.228  1.00 50.69      B    N
ATOM   3260  CD2 HIS B  18      -1.844  48.147  -6.962  1.00 50.64      B    C
ATOM   3261  C   HIS B  18       1.429  49.229  -3.770  1.00 49.16      B    C
ATOM   3262  O   HIS B  18       2.598  48.822  -3.738  1.00 49.03      B    O
ATOM   3263  N   ASN B  19       0.690  49.386  -2.667  1.00 49.15      B    N
ATOM   3264  CA  ASN B  19       1.167  48.868  -1.384  1.00 49.11      B    C
ATOM   3265  CB  ASN B  19       0.276  49.313  -0.205  1.00 49.60      B    C
ATOM   3266  CG  ASN B  19       0.951  49.099   1.176  1.00 51.24      B    C
ATOM   3267  OD1 ASN B  19       0.415  48.415   2.058  1.00 53.59      B    O
ATOM   3268  ND2 ASN B  19       2.123  49.705   1.363  1.00 54.56      B    N
ATOM   3269  C   ASN B  19       1.241  47.332  -1.459  1.00 48.22      B    C
ATOM   3270  O   ASN B  19       0.443  46.685  -2.138  1.00 47.43      B    O
ATOM   3271  N   LEU B  20       2.221  46.772  -0.762  1.00 47.20      B    N
ATOM   3272  CA  LEU B  20       2.393  45.333  -0.689  1.00 46.38      B    C
ATOM   3273  CB  LEU B  20       3.743  45.000  -0.055  1.00 46.97      B    C
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ATOM   3274  CG  LEU B  20       4.896  45.800  -0.684  1.00 48.40      B    C
ATOM   3275  CD1 LEU B  20       6.201  45.666   0.117  1.00 49.54      B    C
ATOM   3276  CD2 LEU B  20       5.076  45.391  -2.158  1.00 48.69      B    C
ATOM   3277  C   LEU B  20       1.235  44.792   0.141  1.00 44.75      B    C
ATOM   3278  O   LEU B  20       1.113  45.092   1.342  1.00 45.26      B    O
ATOM   3279  N   LYS B  21       0.338  44.073  -0.523  1.00 41.97      B    N
ATOM   3280  CA  LYS B  21      -0.740  43.395   0.170  1.00 39.98      B    C
ATOM   3281  CB  LYS B  21      -2.088  44.025  -0.183  1.00 40.54      B    C
ATOM   3282  CG  LYS B  21      -3.225  43.550   0.700  1.00 41.63      B    C
ATOM   3283  CD  LYS B  21      -4.257  44.620   0.878  1.00 43.44      B    C
ATOM   3284  CE  LYS B  21      -5.391  44.131   1.718  1.00 44.82      B    C
ATOM   3285  NZ  LYS B  21      -4.992  44.004   3.147  1.00 47.17      B    N
ATOM   3286  C   LYS B  21      -0.710  41.917  -0.214  1.00 37.09      B    C
ATOM   3287  O   LYS B  21      -0.679  41.588  -1.395  1.00 35.80      B    O
ATOM   3288  N   THR B  22      -0.685  41.045   0.796  1.00 33.91      B    N
ATOM   3289  CA  THR B  22      -0.642  39.592   0.593  1.00 31.44      B    C
ATOM   3290  CB  THR B  22       0.734  39.046   1.030  1.00 31.70      B    C
ATOM   3291  OG1 THR B  22       1.002  39.436   2.387  1.00 31.47      B    O
ATOM   3292  CG2 THR B  22       1.857  39.681   0.211  1.00 31.30      B    C
ATOM   3293  C   THR B  22      -1.739  38.843   1.342  1.00 29.57      B    C
ATOM   3294  O   THR B  22      -1.830  37.617   1.246  1.00 28.17      B    O
ATOM   3295  N   GLU B  23      -2.542  39.576   2.107  1.00 27.46      B    N
ATOM   3296  CA  GLU B  23      -3.672  39.011   2.828  1.00 27.22      B    C
ATOM   3297  CB BGLU B  23      -3.280  38.728   4.282  0.50 27.51      B    C
ATOM   3298  CB AGLU B  23      -3.287  38.646   4.277  0.50 27.17      B    C
ATOM   3299  CG BGLU B  23      -2.826  37.304   4.512  0.50 29.10      B    C
ATOM   3300  CG AGLU B  23      -3.050  39.822   5.223  0.50 27.55      B    C
ATOM   3301  CD BGLU B  23      -2.236  37.062   5.891  0.50 30.84      B    C
ATOM   3302  CD AGLU B  23      -3.020  39.396   6.689  0.50 28.07      B    C
ATOM   3303  OE1BGLU B  23      -1.959  38.040   6.614  0.50 32.02      B    O
ATOM   3304  OE1AGLU B  23      -2.853  38.186   6.954  0.50 28.41      B    O
ATOM   3305  OE2BGLU B  23      -2.054  35.879   6.241  0.50 31.16      B    O
ATOM   3306  OE2AGLU B  23      -3.182  40.264   7.579  0.50 28.60      B    O
ATOM   3307  C   GLU B  23      -4.842  39.988   2.799  1.00 25.94      B    C
ATOM   3308  O   GLU B  23      -4.631  41.199   2.805  1.00 25.17      B    O
ATOM   3309  N   TRP B  24      -6.065  39.462   2.765  1.00 24.57      B    N
ATOM   3310  CA  TRP B  24      -7.264  40.300   2.708  1.00 23.89      B    C
ATOM   3311  CB  TRP B  24      -7.910  40.174   1.304  1.00 23.59      B    C
ATOM   3312  CG  TRP B  24      -7.105  40.786   0.245  1.00 21.71      B    C
ATOM   3313  CD1 TRP B  24      -7.232  42.050  -0.239  1.00 21.02      B    C
ATOM   3314  NE1 TRP B  24      -6.293  42.276  -1.211  1.00 18.62      B    N
ATOM   3315  CE2 TRP B  24      -5.544  41.148  -1.396  1.00 19.02      B    C
ATOM   3316  CD2 TRP B  24      -6.006  40.190  -0.480  1.00 20.72      B    C
ATOM   3317  CE3 TRP B  24      -5.387  38.941  -0.454  1.00 19.49      B    C
ATOM   3318  CZ3 TRP B  24      -4.326  38.694  -1.313  1.00 20.25      B    C
ATOM   3319  CH2 TRP B  24      -3.883  39.662  -2.207  1.00 21.63      B    C
ATOM   3320  CZ2 TRP B  24      -4.477  40.911  -2.257  1.00 22.09      B    C
ATOM   3321  C   TRP B  24      -8.294  39.948   3.789  1.00 23.91      B    C
ATOM   3322  O   TRP B  24      -9.369  39.456   3.467  1.00 22.74      B    O
ATOM   3323  N   PRO B  25      -7.986  40.196   5.070  1.00 24.64      B    N
ATOM   3324  CA  PRO B  25      -8.918  39.850   6.161  1.00 25.12      B    C
ATOM   3325  CB  PRO B  25      -8.176  40.312   7.448  1.00 25.87      B    C
ATOM   3326  CG  PRO B  25      -7.011  41.163   7.002  1.00 26.08      B    C
ATOM   3327  CD  PRO B  25      -6.737  40.807   5.562  1.00 25.49      B    C
ATOM   3328  C   PRO B  25     -10.307  40.520   6.029  1.00 25.18      B    C
ATOM   3329  O   PRO B  25     -11.310  39.978   6.469  1.00 24.94      B    O
ATOM   3330  N   GLU B  26     -10.350  41.668   5.364  1.00 25.43      B    N
ATOM   3331  CA  GLU B  26     -11.581  42.416   5.141  1.00 25.93      B    C
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ATOM   3332  CB  GLU B  26     -11.243  43.829   4.627  1.00 26.70      B    C
ATOM   3333  CG  GLU B  26     -10.690  43.922   3.189  1.00 28.62      B    C
ATOM   3334  CD  GLU B  26      -9.169  43.775   3.077  1.00 29.61      B    C
ATOM   3335  OE1 GLU B  26      -8.535  43.174   3.985  1.00 28.68      B    O
ATOM   3336  OE2 GLU B  26      -8.608  44.252   2.057  1.00 31.71      B    O
ATOM   3337  C   GLU B  26     -12.571  41.705   4.193  1.00 25.60      B    C
ATOM   3338  O   GLU B  26     -13.746  42.060   4.139  1.00 24.75      B    O
ATOM   3339  N   LEU B  27     -12.119  40.672   3.483  1.00 24.52      B    N
ATOM   3340  CA  LEU B  27     -12.957  40.024   2.483  1.00 23.54      B    C
ATOM   3341  CB  LEU B  27     -12.104  39.593   1.287  1.00 23.84      B    C
ATOM   3342  CG  LEU B  27     -11.506  40.722   0.430  1.00 23.08      B    C
ATOM   3343  CD1 LEU B  27     -10.702  40.165  -0.732  1.00 22.31      B    C
ATOM   3344  CD2 LEU B  27     -12.603  41.624  -0.097  1.00 23.37      B    C
ATOM   3345  C   LEU B  27     -13.716  38.829   3.042  1.00 23.75      B    C
ATOM   3346  O   LEU B  27     -14.504  38.205   2.334  1.00 23.33      B    O
ATOM   3347  N   VAL B  28     -13.490  38.504   4.312  1.00 23.89      B    N
ATOM   3348  CA  VAL B  28     -14.143  37.357   4.918  1.00 24.64      B    C
ATOM   3349  CB  VAL B  28     -13.571  37.050   6.359  1.00 24.78      B    C
ATOM   3350  CG1 VAL B  28     -14.359  35.963   7.027  1.00 25.39      B    C
ATOM   3351  CG2 VAL B  28     -12.099  36.634   6.272  1.00 25.78      B    C
ATOM   3352  C   VAL B  28     -15.612  37.694   4.992  1.00 24.75      B    C
ATOM   3353  O   VAL B  28     -15.952  38.791   5.424  1.00 25.68      B    O
ATOM   3354  N   GLY B  29     -16.468  36.797   4.516  1.00 24.86      B    N
ATOM   3355  CA  GLY B  29     -17.916  37.000   4.539  1.00 24.80      B    C
ATOM   3356  C   GLY B  29     -18.493  37.638   3.274  1.00 25.07      B    C
ATOM   3357  O   GLY B  29     -19.692  37.598   3.061  1.00 25.27      B    O
ATOM   3358  N   LYS B  30     -17.630  38.203   2.429  1.00 25.21      B    N
ATOM   3359  CA  LYS B  30     -18.025  38.782   1.146  1.00 24.62      B    C
ATOM   3360  CB  LYS B  30     -16.952  39.780   0.679  1.00 25.65      B    C
ATOM   3361  CG  LYS B  30     -16.716  40.964   1.606  1.00 28.42      B    C
ATOM   3362  CD  LYS B  30     -16.577  42.245   0.785  1.00 34.26      B    C
ATOM   3363  CE  LYS B  30     -16.462  43.527   1.631  1.00 35.92      B    C
ATOM   3364  NZ  LYS B  30     -15.996  43.273   3.011  1.00 37.72      B    N
ATOM   3365  C   LYS B  30     -18.188  37.728   0.065  1.00 23.30      B    C
ATOM   3366  O   LYS B  30     -17.670  36.623   0.166  1.00 22.29      B    O
ATOM   3367  N   SER B  31     -18.884  38.089  -1.001  1.00 21.94      B    N
ATOM   3368  CA  SER B  31     -19.036  37.204  -2.145  1.00 20.89      B    C
ATOM   3369  CB  SER B  31     -20.046  37.776  -3.143  1.00 21.21      B    C
ATOM   3370  OG  SER B  31     -19.519  38.912  -3.815  1.00 20.40      B    O
ATOM   3371  C   SER B  31     -17.726  37.017  -2.865  1.00 19.88      B    C
ATOM   3372  O   SER B  31     -16.828  37.843  -2.800  1.00 18.67      B    O
ATOM   3373  N   VAL B  32     -17.649  35.920  -3.588  1.00 20.34      B    N
ATOM   3374  CA  VAL B  32     -16.487  35.617  -4.393  1.00 20.89      B    C
ATOM   3375  CB BVAL B  32     -16.717  34.256  -5.141  0.50 20.94      B    C
ATOM   3376  CB AVAL B  32     -16.555  34.234  -5.043  0.50 21.07      B    C
ATOM   3377  CG1BVAL B  32     -16.023  34.221  -6.524  0.50 20.85      B    C
ATOM   3378  CG1AVAL B  32     -17.648  34.180  -6.069  0.50 20.79      B    C
ATOM   3379  CG2BVAL B  32     -16.276  33.087  -4.281  0.50 20.73      B    C
ATOM   3380  CG2AVAL B  32     -15.193  33.903  -5.657  0.50 21.36      B    C
ATOM   3381  C   VAL B  32     -16.238  36.732  -5.431  1.00 20.83      B    C
ATOM   3382  O   VAL B  32     -15.100  37.105  -5.681  1.00 20.37      B    O
ATOM   3383  N   GLU B  33     -17.316  37.263  -6.011  1.00 21.19      B    N
ATOM   3384  CA  GLU B  33     -17.205  38.264  -7.072  1.00 21.20      B    C
ATOM   3385  CB  GLU B  33     -18.553  38.478  -7.767  1.00 21.59      B    C
ATOM   3386  CG  GLU B  33     -19.045  37.271  -8.543  1.00 24.67      B    C
ATOM   3387  CD  GLU B  33     -19.799  36.219  -7.708  1.00 29.01      B    C
ATOM   3388  OE1 GLU B  33     -20.001  35.123  -8.275  1.00 36.54      B    O
ATOM   3389  OE2 GLU B  33     -20.187  36.437  -6.517  1.00 27.78      B    O
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ATOM	3390	C	GLU	B	33	-16.688	39.571	-6.497	1.00	20.62	B	C
ATOM	3391	O	GLU	B	33	-15.885	40.255	-7.130	1.00	20.20	B	O
ATOM	3392	N	GLU	B	34	-17.124	39.910	-5.283	1.00	20.61	B	N
ATOM	3393	CA	GLU	B	34	-16.627	41.131	-4.634	1.00	20.97	B	C
ATOM	3394	CB	GLU	B	34	-17.456	41.533	-3.407	1.00	21.10	B	C
ATOM	3395	CG	GLU	B	34	-18.778	42.224	-3.722	1.00	25.82	B	C
ATOM	3396	CD	GLU	B	34	-18.615	43.546	-4.481	1.00	31.16	B	C
ATOM	3397	OE1	GLU	B	34	-17.968	44.484	-3.932	1.00	32.84	B	O
ATOM	3398	OE2	GLU	B	34	-19.135	43.645	-5.626	1.00	33.71	B	O
ATOM	3399	C	GLU	B	34	-15.156	40.951	-4.257	1.00	19.67	B	C
ATOM	3400	O	GLU	B	34	-14.340	41.858	-4.438	1.00	18.91	B	O
ATOM	3401	N	ALA	B	35	-14.809	39.775	-3.765	1.00	19.75	B	N
ATOM	3402	CA	ALA	B	35	-13.414	39.485	-3.401	1.00	19.10	B	C
ATOM	3403	CB	ALA	B	35	-13.311	38.127	-2.749	1.00	19.66	B	C
ATOM	3404	C	ALA	B	35	-12.457	39.581	-4.582	1.00	18.90	B	C
ATOM	3405	O	ALA	B	35	-11.387	40.183	-4.470	1.00	18.82	B	O
ATOM	3406	N	LYS	B	36	-12.839	38.993	-5.716	1.00	18.68	B	N
ATOM	3407	CA	LYS	B	36	-11.991	38.978	-6.894	1.00	18.17	B	C
ATOM	3408	CB	LYS	B	36	-12.659	38.220	-8.063	1.00	18.44	B	C
ATOM	3409	CG	LYS	B	36	-12.714	36.693	-7.928	1.00	19.56	B	C
ATOM	3410	CD	LYS	B	36	-13.304	36.026	-9.159	1.00	20.72	B	C
ATOM	3411	CE	LYS	B	36	-13.194	34.496	-9.136	1.00	22.32	B	C
ATOM	3412	NZ	LYS	B	36	-13.963	33.865	-10.274	1.00	20.54	B	N
ATOM	3413	C	LYS	B	36	-11.648	40.406	-7.316	1.00	17.67	B	C
ATOM	3414	O	LYS	B	36	-10.500	40.694	-7.681	1.00	17.81	B	O
ATOM	3415	N	LYS	B	37	-12.614	41.316	-7.254	1.00	17.52	B	N
ATOM	3416	CA	LYS	B	37	-12.345	42.667	-7.746	1.00	17.89	B	C
ATOM	3417	CB	LYS	B	37	-13.621	43.519	-7.870	1.00	17.35	B	C
ATOM	3418	CG	LYS	B	37	-14.544	43.165	-9.036	1.00	17.43	B	C
ATOM	3419	CD	LYS	B	37	-15.847	44.074	-9.064	1.00	15.06	B	C
ATOM	3420	CE	LYS	B	37	-16.801	43.812	-7.921	1.00	16.48	B	C
ATOM	3421	NZ	LYS	B	37	-18.031	44.685	-7.989	1.00	15.66	B	N
ATOM	3422	C	LYS	B	37	-11.333	43.372	-6.852	1.00	18.04	B	C
ATOM	3423	O	LYS	B	37	-10.499	44.126	-7.354	1.00	18.33	B	O
ATOM	3424	N	VAL	B	38	-11.436	43.174	-5.535	1.00	17.93	B	N
ATOM	3425	CA	VAL	B	38	-10.525	43.824	-4.595	1.00	18.53	B	C
ATOM	3426	CB	VAL	B	38	-11.024	43.636	-3.136	1.00	19.32	B	C
ATOM	3427	CG1	VAL	B	38	-9.975	44.055	-2.128	1.00	21.52	B	C
ATOM	3428	CG2	VAL	B	38	-12.310	44.445	-2.919	1.00	20.73	B	C
ATOM	3429	C	VAL	B	38	-9.122	43.270	-4.742	1.00	18.91	B	C
ATOM	3430	O	VAL	B	38	-8.135	44.013	-4.797	1.00	17.79	B	O
ATOM	3431	N	ILE	B	39	-9.033	41.947	-4.830	1.00	19.11	B	N
ATOM	3432	CA	ILE	B	39	-7.747	41.304	-5.009	1.00	19.64	B	C
ATOM	3433	CB	ILE	B	39	-7.919	39.764	-4.973	1.00	19.43	B	C
ATOM	3434	CG1	ILE	B	39	-8.288	39.324	-3.573	1.00	20.37	B	C
ATOM	3435	CD1	ILE	B	39	-8.994	37.995	-3.564	1.00	21.36	B	C
ATOM	3436	CG2	ILE	B	39	-6.657	39.024	-5.470	1.00	19.76	B	C
ATOM	3437	C	ILE	B	39	-7.077	41.759	-6.287	1.00	19.71	B	C
ATOM	3438	O	ILE	B	39	-5.877	42.087	-6.266	1.00	19.70	B	O
ATOM	3439	N	LEU	B	40	-7.816	41.785	-7.404	1.00	19.22	B	N
ATOM	3440	CA	LEU	B	40	-7.205	42.231	-8.664	1.00	19.62	B	C
ATOM	3441	CB	LEU	B	40	-8.100	41.927	-9.888	1.00	19.18	B	C
ATOM	3442	CG	LEU	B	40	-8.145	40.416	-10.190	1.00	20.23	B	C
ATOM	3443	CD1	LEU	B	40	-9.235	40.047	-11.123	1.00	19.43	B	C
ATOM	3444	CD2	LEU	B	40	-6.799	39.947	-10.725	1.00	21.26	B	C
ATOM	3445	C	LEU	B	40	-6.840	43.716	-8.608	1.00	19.20	B	C
ATOM	3446	O	LEU	B	40	-5.939	44.144	-9.300	1.00	19.48	B	O
ATOM	3447	N	GLN	B	41	-7.553	44.494	-7.803	1.00	19.70	B	N

ATOM	3448	CA	GLN	B	41	-7.216	45.914	-7.622	1.00	20.69	B	C
ATOM	3449	CB	GLN	B	41	-8.286	46.641	-6.813	1.00	20.30	B	C
ATOM	3450	CG	GLN	B	41	-8.068	48.173	-6.731	1.00	20.90	B	C
ATOM	3451	CD	GLN	B	41	-8.159	48.842	-8.083	1.00	21.54	B	C
ATOM	3452	OE1	GLN	B	41	-9.070	48.529	-8.858	1.00	23.88	B	O
ATOM	3453	NE2	GLN	B	41	-7.224	49.762	-8.384	1.00	20.95	B	N
ATOM	3454	C	GLN	B	41	-5.880	46.050	-6.906	1.00	22.10	B	C
ATOM	3455	O	GLN	B	41	-5.105	46.941	-7.213	1.00	22.64	B	O
ATOM	3456	N	ASP	B	42	-5.625	45.149	-5.955	1.00	22.70	B	N
ATOM	3457	CA	ASP	B	42	-4.396	45.178	-5.161	1.00	23.28	B	C
ATOM	3458	CB	ASP	B	42	-4.654	44.531	-3.800	1.00	22.77	B	C
ATOM	3459	CG	ASP	B	42	-5.531	45.369	-2.928	1.00	24.12	B	C
ATOM	3460	OD1	ASP	B	42	-5.619	46.599	-3.174	1.00	27.20	B	O
ATOM	3461	OD2	ASP	B	42	-6.206	44.899	-1.991	1.00	25.78	B	O
ATOM	3462	C	ASP	B	42	-3.273	44.438	-5.859	1.00	23.19	B	C
ATOM	3463	O	ASP	B	42	-2.103	44.761	-5.700	1.00	24.27	B	O
ATOM	3464	N	LYS	B	43	-3.629	43.444	-6.655	1.00	22.96	B	N
ATOM	3465	CA	LYS	B	43	-2.634	42.541	-7.203	1.00	23.10	B	C
ATOM	3466	CB	LYS	B	43	-2.508	41.291	-6.299	1.00	23.07	B	C
ATOM	3467	CG	LYS	B	43	-1.376	40.306	-6.701	1.00	23.16	B	C
ATOM	3468	CD	LYS	B	43	-1.348	39.100	-5.750	1.00	24.15	B	C
ATOM	3469	CE	LYS	B	43	-0.391	37.996	-6.217	1.00	25.40	B	C
ATOM	3470	NZ	LYS	B	43	1.031	38.403	-6.170	1.00	25.72	B	N
ATOM	3471	C	LYS	B	43	-3.067	42.157	-8.593	1.00	23.00	B	C
ATOM	3472	O	LYS	B	43	-3.672	41.107	-8.782	1.00	22.17	B	O
ATOM	3473	N	PRO	B	44	-2.772	43.010	-9.571	1.00	24.07	B	N
ATOM	3474	CA	PRO	B	44	-3.282	42.826	-10.948	1.00	24.35	B	C
ATOM	3475	CB	PRO	B	44	-2.632	43.985	-11.735	1.00	24.65	B	C
ATOM	3476	CG	PRO	B	44	-2.197	44.997	-10.702	1.00	25.50	B	C
ATOM	3477	CD	PRO	B	44	-1.960	44.238	-9.415	1.00	24.73	B	C
ATOM	3478	C	PRO	B	44	-2.929	41.486	-11.583	1.00	24.65	B	C
ATOM	3479	O	PRO	B	44	-3.680	40.967	-12.409	1.00	25.49	B	O
ATOM	3480	N	GLU	B	45	-1.778	40.935	-11.206	1.00	25.20	B	N
ATOM	3481	CA	GLU	B	45	-1.310	39.651	-11.725	1.00	25.70	B	C
ATOM	3482	CB	GLU	B	45	0.226	39.599	-11.602	1.00	26.83	B	C
ATOM	3483	CG	GLU	B	45	0.764	39.243	-10.206	1.00	28.74	B	C
ATOM	3484	CD	GLU	B	45	0.925	40.423	-9.262	1.00	32.92	B	C
ATOM	3485	OE1	GLU	B	45	1.667	40.252	-8.253	1.00	34.10	B	O
ATOM	3486	OE2	GLU	B	45	0.316	41.511	-9.488	1.00	33.16	B	O
ATOM	3487	C	GLU	B	45	-1.945	38.404	-11.048	1.00	25.32	B	C
ATOM	3488	O	GLU	B	45	-1.679	37.270	-11.452	1.00	25.52	B	O
ATOM	3489	N	ALA	B	46	-2.788	38.593	-10.034	1.00	24.59	B	N
ATOM	3490	CA	ALA	B	46	-3.327	37.441	-9.309	1.00	23.90	B	C
ATOM	3491	CB	ALA	B	46	-4.271	37.895	-8.229	1.00	23.95	B	C
ATOM	3492	C	ALA	B	46	-4.015	36.426	-10.216	1.00	23.75	B	C
ATOM	3493	O	ALA	B	46	-4.777	36.788	-11.103	1.00	22.67	B	O
ATOM	3494	N	GLN	B	47	-3.717	35.150	-9.982	1.00	23.77	B	N
ATOM	3495	CA	GLN	B	47	-4.438	34.035	-10.568	1.00	24.59	B	C
ATOM	3496	CB	GLN	B	47	-3.479	32.976	-11.105	1.00	25.29	B	C
ATOM	3497	CG	GLN	B	47	-2.425	33.498	-12.080	1.00	28.88	B	C
ATOM	3498	CD	GLN	B	47	-3.025	33.975	-13.393	1.00	35.56	B	C
ATOM	3499	OE1	GLN	B	47	-3.624	33.176	-14.144	1.00	40.01	B	O
ATOM	3500	NE2	GLN	B	47	-2.869	35.278	-13.686	1.00	38.46	B	N
ATOM	3501	C	GLN	B	47	-5.298	33.425	-9.460	1.00	23.84	B	C
ATOM	3502	O	GLN	B	47	-4.786	32.790	-8.517	1.00	24.12	B	O
ATOM	3503	N	ILE	B	48	-6.597	33.644	-9.559	1.00	22.91	B	N
ATOM	3504	CA	ILE	B	48	-7.502	33.329	-8.463	1.00	23.01	B	C
ATOM	3505	CB	ILE	B	48	-8.486	34.462	-8.235	1.00	22.88	B	C

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ATOM   3506  CG1 ILE B  48      -7.708  35.747  -7.988  1.00 22.10      B    C
ATOM   3507  CD1 ILE B  48      -8.568  36.992  -7.917  1.00 22.38      B    C
ATOM   3508  CG2 ILE B  48      -9.391  34.161  -7.036  1.00 21.57      B    C
ATOM   3509  C   ILE B  48      -8.230  32.047  -8.746  1.00 23.69      B    C
ATOM   3510  O   ILE B  48      -8.685  31.820  -9.877  1.00 23.31      B    O
ATOM   3511  N   ILE B  49      -8.277  31.206  -7.716  1.00 23.55      B    N
ATOM   3512  CA  ILE B  49      -8.894  29.894  -7.746  1.00 24.95      B    C
ATOM   3513  CB  ILE B  49      -7.803  28.812  -7.480  1.00 26.22      B    C
ATOM   3514  CG1 ILE B  49      -6.723  28.868  -8.575  1.00 29.02      B    C
ATOM   3515  CD1 ILE B  49      -7.264  28.733  -9.982  1.00 29.18      B    C
ATOM   3516  CG2 ILE B  49      -8.409  27.422  -7.364  1.00 28.74      B    C
ATOM   3517  C   ILE B  49      -9.903  29.851  -6.610  1.00 23.74      B    C
ATOM   3518  O   ILE B  49      -9.620  30.348  -5.511  1.00 24.09      B    O
ATOM   3519  N   VAL B  50     -11.045  29.224  -6.847  1.00 22.75      B    N
ATOM   3520  CA  VAL B  50     -12.088  29.110  -5.838  1.00 22.00      B    C
ATOM   3521  CB  VAL B  50     -13.441  29.682  -6.364  1.00 21.55      B    C
ATOM   3522  CG1 VAL B  50     -14.583  29.378  -5.388  1.00 22.01      B    C
ATOM   3523  CG2 VAL B  50     -13.338  31.190  -6.581  1.00 21.04      B    C
ATOM   3524  C   VAL B  50     -12.273  27.639  -5.439  1.00 21.99      B    C
ATOM   3525  O   VAL B  50     -12.375  26.780  -6.291  1.00 21.98      B    O
ATOM   3526  N   LEU B  51     -12.318  27.363  -4.141  1.00 21.70      B    N
ATOM   3527  CA  LEU B  51     -12.460  26.003  -3.643  1.00 22.26      B    C
ATOM   3528  CB  LEU B  51     -11.110  25.407  -3.219  1.00 22.70      B    C
ATOM   3529  CG  LEU B  51     -10.067  25.113  -4.267  1.00 25.11      B    C
ATOM   3530  CD1 LEU B  51      -8.762  24.764  -3.495  1.00 25.85      B    C
ATOM   3531  CD2 LEU B  51     -10.513  23.968  -5.183  1.00 27.79      B    C
ATOM   3532  C   LEU B  51     -13.312  25.997  -2.406  1.00 21.80      B    C
ATOM   3533  O   LEU B  51     -13.289  26.962  -1.646  1.00 21.46      B    O
ATOM   3534  N   PRO B  52     -14.006  24.886  -2.163  1.00 21.76      B    N
ATOM   3535  CA  PRO B  52     -14.750  24.709  -0.921  1.00 22.13      B    C
ATOM   3536  CB  PRO B  52     -15.340  23.290  -1.071  1.00 23.06      B    C
ATOM   3537  CG  PRO B  52     -15.389  23.059  -2.525  1.00 22.20      B    C
ATOM   3538  CD  PRO B  52     -14.145  23.724  -3.058  1.00 22.25      B    C
ATOM   3539  C   PRO B  52     -13.836  24.809   0.290  1.00 22.83      B    C
ATOM   3540  O   PRO B  52     -12.682  24.367   0.252  1.00 22.05      B    O
ATOM   3541  N   VAL B  53     -14.340  25.400   1.365  1.00 23.43      B    N
ATOM   3542  CA  VAL B  53     -13.579  25.504   2.581  1.00 23.96      B    C
ATOM   3543  CB  VAL B  53     -14.297  26.368   3.643  1.00 24.41      B    C
ATOM   3544  CG1 VAL B  53     -15.583  25.692   4.134  1.00 25.13      B    C
ATOM   3545  CG2 VAL B  53     -13.360  26.671   4.805  1.00 25.93      B    C
ATOM   3546  C   VAL B  53     -13.324  24.083   3.068  1.00 24.12      B    C
ATOM   3547  O   VAL B  53     -14.153  23.193   2.859  1.00 24.69      B    O
ATOM   3548  N   GLY B  54     -12.158  23.867   3.657  1.00 22.87      B    N
ATOM   3549  CA  GLY B  54     -11.765  22.548   4.117  1.00 22.48      B    C
ATOM   3550  C   GLY B  54     -11.067  21.662   3.092  1.00 21.22      B    C
ATOM   3551  O   GLY B  54     -10.597  20.606   3.453  1.00 21.63      B    O
ATOM   3552  N   THR B  55     -10.977  22.091   1.837  1.00 20.24      B    N
ATOM   3553  CA  THR B  55     -10.295  21.324   0.809  1.00 19.46      B    C
ATOM   3554  CB  THR B  55     -10.469  22.006  -0.573  1.00 19.86      B    C
ATOM   3555  OG1 THR B  55     -11.866  22.158  -0.875  1.00 22.41      B    O
ATOM   3556  CG2 THR B  55      -9.957  21.139  -1.701  1.00 19.94      B    C
ATOM   3557  C   THR B  55      -8.788  21.125   1.077  1.00 17.93      B    C
ATOM   3558  O   THR B  55      -8.057  22.042   1.417  1.00 16.91      B    O
ATOM   3559  N   ILE B  56      -8.336  19.911   0.849  1.00 17.04      B    N
ATOM   3560  CA  ILE B  56      -6.929  19.571   0.943  1.00 16.44      B    C
ATOM   3561  CB  ILE B  56      -6.800  18.076   1.232  1.00 15.71      B    C
ATOM   3562  CG1 ILE B  56      -7.439  17.782   2.600  1.00 17.41      B    C
ATOM   3563  CD1 ILE B  56      -7.353  16.319   3.098  1.00 17.17      B    C
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ATOM	3564	CG2	ILE	B	56	-5.347	17.684	1.247	1.00	16.77	B	C
ATOM	3565	C	ILE	B	56	-6.217	19.981	-0.336	1.00	16.51	B	C
ATOM	3566	O	ILE	B	56	-6.701	19.691	-1.434	1.00	17.03	B	O
ATOM	3567	N	VAL	B	57	-5.088	20.678	-0.203	1.00	15.94	B	N
ATOM	3568	CA	VAL	B	57	-4.342	21.200	-1.361	1.00	16.45	B	C
ATOM	3569	CB	VAL	B	57	-4.511	22.726	-1.488	1.00	16.21	B	C
ATOM	3570	CG1	VAL	B	57	-6.012	23.092	-1.672	1.00	16.73	B	C
ATOM	3571	CG2	VAL	B	57	-3.991	23.435	-0.236	1.00	18.16	B	C
ATOM	3572	C	VAL	B	57	-2.853	20.910	-1.205	1.00	16.63	B	C
ATOM	3573	O	VAL	B	57	-2.393	20.624	-0.099	1.00	16.42	B	O
ATOM	3574	N	THR	B	58	-2.106	20.982	-2.299	1.00	17.06	B	N
ATOM	3575	CA	THR	B	58	-0.658	20.801	-2.247	1.00	16.63	B	C
ATOM	3576	CB	THR	B	58	-0.069	20.712	-3.654	1.00	17.18	B	C
ATOM	3577	OG1	THR	B	58	-0.660	21.718	-4.494	1.00	15.16	B	O
ATOM	3578	CG2	THR	B	58	-0.423	19.426	-4.292	1.00	19.58	B	C
ATOM	3579	C	THR	B	58	-0.093	22.017	-1.536	1.00	16.72	B	C
ATOM	3580	O	THR	B	58	-0.756	23.071	-1.492	1.00	16.30	B	O
ATOM	3581	N	MET	B	59	1.103	21.885	-0.960	1.00	16.38	B	N
ATOM	3582	CA	MET	B	59	1.692	22.982	-0.180	1.00	16.07	B	C
ATOM	3583	CB	MET	B	59	1.960	22.552	1.254	1.00	15.92	B	C
ATOM	3584	CG	MET	B	59	0.668	22.365	2.012	1.00	16.14	B	C
ATOM	3585	SD	MET	B	59	-0.197	23.961	2.251	1.00	17.09	B	S
ATOM	3586	CE	MET	B	59	-1.612	23.424	3.218	1.00	17.23	B	C
ATOM	3587	C	MET	B	59	2.911	23.607	-0.816	1.00	15.83	B	C
ATOM	3588	O	MET	B	59	3.884	23.983	-0.134	1.00	15.99	B	O
ATOM	3589	N	GLU	B	60	2.837	23.794	-2.127	1.00	15.11	B	N
ATOM	3590	CA	GLU	B	60	3.838	24.609	-2.795	1.00	15.22	B	C
ATOM	3591	CB	GLU	B	60	4.155	24.079	-4.187	1.00	15.39	B	C
ATOM	3592	CG	GLU	B	60	3.299	24.609	-5.334	1.00	15.29	B	C
ATOM	3593	CD	GLU	B	60	1.845	24.166	-5.270	1.00	19.22	B	C
ATOM	3594	OE1	GLU	B	60	1.435	23.486	-4.308	1.00	18.05	B	O
ATOM	3595	OE2	GLU	B	60	1.087	24.526	-6.195	1.00	18.12	B	O
ATOM	3596	C	GLU	B	60	3.344	26.081	-2.771	1.00	15.50	B	C
ATOM	3597	O	GLU	B	60	2.133	26.356	-2.798	1.00	15.17	B	O
ATOM	3598	N	TYR	B	61	4.292	27.011	-2.721	1.00	16.00	B	N
ATOM	3599	CA	TYR	B	61	3.982	28.431	-2.654	1.00	17.37	B	C
ATOM	3600	CB	TYR	B	61	4.938	29.138	-1.699	1.00	17.67	B	C
ATOM	3601	CG	TYR	B	61	4.671	30.623	-1.493	1.00	18.81	B	C
ATOM	3602	CD1	TYR	B	61	5.474	31.572	-2.103	1.00	21.63	B	C
ATOM	3603	CE1	TYR	B	61	5.233	32.895	-1.943	1.00	21.96	B	C
ATOM	3604	CZ	TYR	B	61	4.207	33.299	-1.134	1.00	22.89	B	C
ATOM	3605	OH	TYR	B	61	4.007	34.644	-0.972	1.00	29.91	B	O
ATOM	3606	CE2	TYR	B	61	3.407	32.394	-0.507	1.00	20.81	B	C
ATOM	3607	CD2	TYR	B	61	3.637	31.059	-0.697	1.00	19.36	B	C
ATOM	3608	C	TYR	B	61	4.067	29.037	-4.048	1.00	18.22	B	C
ATOM	3609	O	TYR	B	61	5.126	29.041	-4.654	1.00	18.04	B	O
ATOM	3610	N	ARG	B	62	2.943	29.531	-4.564	1.00	19.75	B	N
ATOM	3611	CA	ARG	B	62	2.938	30.226	-5.861	1.00	21.16	B	C
ATOM	3612	CB	ARG	B	62	1.909	29.625	-6.814	1.00	21.92	B	C
ATOM	3613	CG	ARG	B	62	2.189	28.185	-7.196	1.00	25.65	B	C
ATOM	3614	CD	ARG	B	62	1.385	27.694	-8.421	1.00	29.39	B	C
ATOM	3615	NE	ARG	B	62	1.516	26.235	-8.639	1.00	32.04	B	N
ATOM	3616	CZ	ARG	B	62	0.982	25.593	-9.675	1.00	33.94	B	C
ATOM	3617	NH1	ARG	B	62	1.129	24.287	-9.798	1.00	37.42	B	N
ATOM	3618	NH2	ARG	B	62	0.292	26.255	-10.586	1.00	34.66	B	N
ATOM	3619	C	ARG	B	62	2.619	31.687	-5.652	1.00	21.86	B	C
ATOM	3620	O	ARG	B	62	1.491	32.033	-5.296	1.00	21.34	B	O
ATOM	3621	N	ILE	B	63	3.609	32.547	-5.894	1.00	23.01	B	N

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ATOM   3622  CA   ILE B  63       3.503  33.950  -5.502  1.00 24.71      B    C
ATOM   3623  CB   ILE B  63       4.824  34.707  -5.709  1.00 25.05      B    C
ATOM   3624  CG1  ILE B  63       4.790  36.033  -4.919  1.00 28.83      B    C
ATOM   3625  CD1  ILE B  63       6.158  36.609  -4.546  1.00 31.61      B    C
ATOM   3626  CG2  ILE B  63       5.047  34.966  -7.207  1.00 26.58      B    C
ATOM   3627  C    ILE B  63       2.367  34.699  -6.216  1.00 24.34      B    C
ATOM   3628  O    ILE B  63       1.860  35.675  -5.672  1.00 25.45      B    O
ATOM   3629  N    ASP B  64       1.961  34.240  -7.398  1.00 24.15      B    N
ATOM   3630  CA   ASP B  64       0.901  34.919  -8.153  1.00 24.63      B    C
ATOM   3631  CB BASP B  64       1.214  34.889  -9.664  0.40 24.94      B    C
ATOM   3632  CB AASP B  64       1.201  34.873  -9.650  0.60 24.96      B    C
ATOM   3633  CG BASP B  64       0.987  33.514 -10.307  0.40 25.65      B    C
ATOM   3634  CG AASP B  64       2.403  35.712 -10.026  0.60 25.91      B    C
ATOM   3635  OD1BASP B  64       0.745  33.465 -11.536  0.40 27.17      B    O
ATOM   3636  OD1AASP B  64       3.136  35.290 -10.950  0.60 27.52      B    O
ATOM   3637  OD2BASP B  64       1.054  32.426  -9.686  0.40 28.49      B    O
ATOM   3638  OD2AASP B  64       2.704  36.782  -9.439  0.60 26.67      B    O
ATOM   3639  C    ASP B  64      -0.514  34.361  -7.896  1.00 24.47      B    C
ATOM   3640  O    ASP B  64      -1.515  34.928  -8.392  1.00 24.83      B    O
ATOM   3641  N    ARG B  65      -0.601  33.269  -7.136  1.00 21.92      B    N
ATOM   3642  CA   ARG B  65      -1.876  32.615  -6.893  1.00 21.12      B    C
ATOM   3643  CB   ARG B  65      -1.677  31.101  -6.737  1.00 19.95      B    C
ATOM   3644  CG   ARG B  65      -2.946  30.305  -6.463  1.00 18.99      B    C
ATOM   3645  CD   ARG B  65      -2.730  28.808  -6.572  1.00 19.09      B    C
ATOM   3646  NE   ARG B  65      -1.784  28.369  -5.554  1.00 18.66      B    N
ATOM   3647  CZ   ARG B  65      -1.130  27.214  -5.534  1.00 19.41      B    C
ATOM   3648  NH1  ARG B  65      -1.279  26.300  -6.470  1.00 19.74      B    N
ATOM   3649  NH2  ARG B  65      -0.311  26.963  -4.522  1.00 21.82      B    N
ATOM   3650  C    ARG B  65      -2.556  33.168  -5.662  1.00 20.36      B    C
ATOM   3651  O    ARG B  65      -1.896  33.515  -4.682  1.00 21.06      B    O
ATOM   3652  N    VAL B  66      -3.875  33.284  -5.727  1.00 20.04      B    N
ATOM   3653  CA   VAL B  66      -4.692  33.540  -4.560  1.00 19.79      B    C
ATOM   3654  CB   VAL B  66      -5.266  34.962  -4.510  1.00 19.88      B    C
ATOM   3655  CG1  VAL B  66      -6.036  35.160  -3.204  1.00 21.06      B    C
ATOM   3656  CG2  VAL B  66      -4.194  36.004  -4.607  1.00 20.96      B    C
ATOM   3657  C    VAL B  66      -5.846  32.525  -4.551  1.00 20.19      B    C
ATOM   3658  O    VAL B  66      -6.733  32.512  -5.444  1.00 20.12      B    O
ATOM   3659  N    ARG B  67      -5.832  31.654  -3.557  1.00 20.01      B    N
ATOM   3660  CA   ARG B  67      -6.916  30.713  -3.394  1.00 20.45      B    C
ATOM   3661  CB   ARG B  67      -6.416  29.437  -2.740  1.00 20.71      B    C
ATOM   3662  CG   ARG B  67      -5.572  28.538  -3.626  1.00 21.28      B    C
ATOM   3663  CD   ARG B  67      -5.471  27.144  -3.016  1.00 23.63      B    C
ATOM   3664  NE   ARG B  67      -4.539  26.204  -3.632  1.00 22.50      B    N
ATOM   3665  CZ   ARG B  67      -3.326  25.921  -3.160  1.00 24.19      B    C
ATOM   3666  NH1  ARG B  67      -2.589  24.992  -3.759  1.00 22.65      B    N
ATOM   3667  NH2  ARG B  67      -2.837  26.571  -2.106  1.00 22.06      B    N
ATOM   3668  C    ARG B  67      -8.001  31.368  -2.543  1.00 20.49      B    C
ATOM   3669  O    ARG B  67      -7.704  31.990  -1.529  1.00 20.17      B    O
ATOM   3670  N    LEU B  68      -9.255  31.253  -2.970  1.00 20.39      B    N
ATOM   3671  CA   LEU B  68     -10.373  31.705  -2.148  1.00 21.05      B    C
ATOM   3672  CB   LEU B  68     -11.323  32.604  -2.957  1.00 21.11      B    C
ATOM   3673  CG   LEU B  68     -10.701  33.830  -3.627  1.00 21.59      B    C
ATOM   3674  CD1  LEU B  68     -11.745  34.523  -4.508  1.00 22.82      B    C
ATOM   3675  CD2  LEU B  68     -10.187  34.785  -2.595  1.00 22.44      B    C
ATOM   3676  C    LEU B  68     -11.132  30.493  -1.648  1.00 21.12      B    C
ATOM   3677  O    LEU B  68     -11.663  29.709  -2.432  1.00 21.87      B    O
ATOM   3678  N    PHE B  69     -11.209  30.345  -0.345  1.00 21.61      B    N
ATOM   3679  CA   PHE B  69     -11.937  29.226   0.233  1.00 21.97      B    C
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ATOM	3680	CB	PHE	B	69	-11.151	28.647	1.422	1.00	22.17	B	C
ATOM	3681	CG	PHE	B	69	-9.896	27.905	1.028	1.00	19.89	B	C
ATOM	3682	CD1	PHE	B	69	-9.938	26.557	0.737	1.00	21.41	B	C
ATOM	3683	CE1	PHE	B	69	-8.788	25.862	0.370	1.00	20.29	B	C
ATOM	3684	CZ	PHE	B	69	-7.598	26.525	0.290	1.00	21.78	B	C
ATOM	3685	CE2	PHE	B	69	-7.542	27.879	0.575	1.00	21.52	B	C
ATOM	3686	CD2	PHE	B	69	-8.691	28.557	0.950	1.00	19.33	B	C
ATOM	3687	C	PHE	B	69	-13.321	29.725	0.664	1.00	23.11	B	C
ATOM	3688	O	PHE	B	69	-13.414	30.651	1.506	1.00	22.87	B	O
ATOM	3689	N	VAL	B	70	-14.371	29.105	0.111	1.00	24.00	B	N
ATOM	3690	CA	VAL	B	70	-15.755	29.578	0.289	1.00	25.82	B	C
ATOM	3691	CB	VAL	B	70	-16.442	29.958	-1.054	1.00	25.72	B	C
ATOM	3692	CG1	VAL	B	70	-15.686	31.063	-1.756	1.00	26.70	B	C
ATOM	3693	CG2	VAL	B	70	-16.599	28.756	-1.958	1.00	26.63	B	C
ATOM	3694	C	VAL	B	70	-16.691	28.602	0.996	1.00	26.63	B	C
ATOM	3695	O	VAL	B	70	-16.532	27.380	0.899	1.00	27.14	B	O
ATOM	3696	N	ASP	B	71	-17.664	29.155	1.714	1.00	27.52	B	N
ATOM	3697	CA	ASP	B	71	-18.686	28.352	2.399	1.00	29.00	B	C
ATOM	3698	CB	ASP	B	71	-19.247	29.132	3.591	1.00	28.91	B	C
ATOM	3699	CG	ASP	B	71	-20.019	30.392	3.171	1.00	28.74	B	C
ATOM	3700	OD1	ASP	B	71	-20.161	31.290	4.018	1.00	29.94	B	O
ATOM	3701	OD2	ASP	B	71	-20.509	30.572	2.032	1.00	27.69	B	O
ATOM	3702	C	ASP	B	71	-19.796	27.931	1.413	1.00	30.37	B	C
ATOM	3703	O	ASP	B	71	-19.646	28.098	0.217	1.00	29.90	B	O
ATOM	3704	N	LYS	B	72	-20.898	27.376	1.906	1.00	33.42	B	N
ATOM	3705	CA	LYS	B	72	-21.949	26.822	1.022	1.00	34.98	B	C
ATOM	3706	CB	LYS	B	72	-22.951	26.004	1.834	1.00	35.44	B	C
ATOM	3707	CG	LYS	B	72	-22.190	24.925	2.916	0.00	40.00	B	C
ATOM	3708	CD	LYS	B	72	-22.489	23.435	2.595	0.00	40.00	B	C
ATOM	3709	CE	LYS	B	72	-21.240	22.528	2.667	0.00	40.00	B	C
ATOM	3710	NZ	LYS	B	72	-21.120	21.662	1.456	0.00	40.00	B	N
ATOM	3711	C	LYS	B	72	-22.709	27.904	0.261	1.00	36.38	B	C
ATOM	3712	O	LYS	B	72	-23.332	27.627	-0.766	1.00	37.77	B	O
ATOM	3713	N	LEU	B	73	-22.640	29.138	0.753	1.00	37.07	B	N
ATOM	3714	CA	LEU	B	73	-23.306	30.286	0.114	1.00	37.22	B	C
ATOM	3715	CB	LEU	B	73	-23.759	31.265	1.201	1.00	37.50	B	C
ATOM	3716	CG	LEU	B	73	-24.711	30.678	2.254	1.00	40.20	B	C
ATOM	3717	CD1	LEU	B	73	-25.387	31.796	3.053	1.00	41.53	B	C
ATOM	3718	CD2	LEU	B	73	-25.782	29.775	1.612	1.00	41.89	B	C
ATOM	3719	C	LEU	B	73	-22.406	31.008	-0.890	1.00	36.59	B	C
ATOM	3720	O	LEU	B	73	-22.781	32.029	-1.482	1.00	36.18	B	O
ATOM	3721	N	ASP	B	74	-21.203	30.468	-1.076	1.00	36.33	B	N
ATOM	3722	CA	ASP	B	74	-20.192	31.084	-1.923	1.00	35.65	B	C
ATOM	3723	CB	ASP	B	74	-20.709	31.252	-3.342	1.00	36.81	B	C
ATOM	3724	CG	ASP	B	74	-20.063	30.283	-4.286	1.00	40.36	B	C
ATOM	3725	OD1	ASP	B	74	-19.429	30.756	-5.259	1.00	45.75	B	O
ATOM	3726	OD2	ASP	B	74	-20.108	29.032	-4.101	1.00	45.61	B	O
ATOM	3727	C	ASP	B	74	-19.646	32.399	-1.381	1.00	33.94	B	C
ATOM	3728	O	ASP	B	74	-19.147	33.249	-2.136	1.00	34.59	B	O
ATOM	3729	N	ASN	B	75	-19.696	32.546	-0.066	1.00	31.85	B	N
ATOM	3730	CA	ASN	B	75	-19.000	33.634	0.597	1.00	30.66	B	C
ATOM	3731	CB	ASN	B	75	-19.877	34.185	1.714	1.00	30.45	B	C
ATOM	3732	CG	ASN	B	75	-21.170	34.793	1.176	1.00	30.77	B	C
ATOM	3733	OD1	ASN	B	75	-21.169	35.401	0.102	1.00	30.57	B	O
ATOM	3734	ND2	ASN	B	75	-22.275	34.615	1.907	1.00	30.32	B	N
ATOM	3735	C	ASN	B	75	-17.628	33.213	1.127	1.00	29.26	B	C
ATOM	3736	O	ASN	B	75	-17.433	32.073	1.553	1.00	29.07	B	O
ATOM	3737	N	ILE	B	76	-16.685	34.143	1.086	1.00	27.83	B	N

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ATOM   3738  CA  ILE B  76     -15.337  33.893   1.540  1.00 26.88      B    C
ATOM   3739  CB  ILE B  76     -14.511  35.182   1.455  1.00 26.51      B    C
ATOM   3740  CG1 ILE B  76     -14.474  35.737   0.020  1.00 26.61      B    C
ATOM   3741  CD1 ILE B  76     -14.130  34.728  -1.039  1.00 26.87      B    C
ATOM   3742  CG2 ILE B  76     -13.137  34.927   1.993  1.00 25.62      B    C
ATOM   3743  C   ILE B  76     -15.401  33.382   2.993  1.00 26.59      B    C
ATOM   3744  O   ILE B  76     -15.994  34.017   3.838  1.00 26.12      B    O
ATOM   3745  N   ALA B  77     -14.795  32.237   3.263  1.00 26.58      B    N
ATOM   3746  CA  ALA B  77     -14.899  31.582   4.576  1.00 26.79      B    C
ATOM   3747  CB  ALA B  77     -15.129  30.088   4.386  1.00 26.56      B    C
ATOM   3748  C   ALA B  77     -13.670  31.815   5.467  1.00 26.89      B    C
ATOM   3749  O   ALA B  77     -13.764  31.751   6.677  1.00 27.73      B    O
ATOM   3750  N   GLU B  78     -12.518  32.072   4.871  1.00 26.32      B    N
ATOM   3751  CA  GLU B  78     -11.355  32.446   5.647  1.00 26.33      B    C
ATOM   3752  CB  GLU B  78     -10.508  31.216   6.041  1.00 26.80      B    C
ATOM   3753  CG  GLU B  78     -10.106  30.290   4.921  1.00 27.82      B    C
ATOM   3754  CD  GLU B  78      -9.956  28.827   5.352  1.00 28.92      B    C
ATOM   3755  OE1 GLU B  78      -9.785  28.493   6.559  1.00 36.40      B    O
ATOM   3756  OE2 GLU B  78     -10.001  27.977   4.472  1.00 28.50      B    O
ATOM   3757  C   GLU B  78     -10.530  33.478   4.895  1.00 25.94      B    C
ATOM   3758  O   GLU B  78     -10.807  33.805   3.712  1.00 25.71      B    O
ATOM   3759  N   VAL B  79      -9.527  33.996   5.594  1.00 24.85      B    N
ATOM   3760  CA  VAL B  79      -8.712  35.088   5.102  1.00 24.88      B    C
ATOM   3761  CB  VAL B  79      -7.692  35.578   6.167  1.00 25.77      B    C
ATOM   3762  CG1 VAL B  79      -6.814  36.672   5.583  1.00 25.38      B    C
ATOM   3763  CG2 VAL B  79      -8.396  36.073   7.456  1.00 26.10      B    C
ATOM   3764  C   VAL B  79      -7.957  34.652   3.835  1.00 24.07      B    C
ATOM   3765  O   VAL B  79      -7.137  33.742   3.883  1.00 23.32      B    O
ATOM   3766  N   PRO B  80      -8.275  35.271   2.699  1.00 23.27      B    N
ATOM   3767  CA  PRO B  80      -7.533  35.029   1.466  1.00 22.93      B    C
ATOM   3768  CB  PRO B  80      -8.296  35.856   0.426  1.00 23.15      B    C
ATOM   3769  CG  PRO B  80      -9.645  36.042   1.005  1.00 23.83      B    C
ATOM   3770  CD  PRO B  80      -9.404  36.194   2.480  1.00 23.67      B    C
ATOM   3771  C   PRO B  80      -6.101  35.512   1.601  1.00 22.05      B    C
ATOM   3772  O   PRO B  80      -5.891  36.588   2.136  1.00 20.76      B    O
ATOM   3773  N   ARG B  81      -5.147  34.691   1.190  1.00 21.54      B    N
ATOM   3774  CA  ARG B  81      -3.765  35.135   1.074  1.00 22.93      B    C
ATOM   3775  CB BARG B  81      -2.937  34.683   2.298  0.40 22.99      B    C
ATOM   3776  CB AARG B  81      -2.865  34.764   2.275  0.60 23.27      B    C
ATOM   3777  CG BARG B  81      -3.684  34.672   3.645  0.40 24.27      B    C
ATOM   3778  CG AARG B  81      -3.278  33.619   3.175  0.60 25.79      B    C
ATOM   3779  CD BARG B  81      -2.996  33.818   4.744  0.40 26.79      B    C
ATOM   3780  CD AARG B  81      -2.615  33.723   4.575  0.60 27.67      B    C
ATOM   3781  NE BARG B  81      -3.975  33.234   5.664  0.40 28.96      B    N
ATOM   3782  NE AARG B  81      -3.283  32.907   5.581  0.60 29.38      B    N
ATOM   3783  CZ BARG B  81      -4.567  32.053   5.508  0.40 29.28      B    C
ATOM   3784  CZ AARG B  81      -3.934  33.381   6.642  0.60 30.17      B    C
ATOM   3785 NH1BARG B  81      -4.284  31.274   4.471  0.40 31.06      B    N
ATOM   3786 NH1AARG B  81      -4.020  34.680   6.867  0.60 31.08      B    N
ATOM   3787 NH2BARG B  81      -5.448  31.645   6.408  0.40 30.62      B    N
ATOM   3788 NH2AARG B  81      -4.510  32.545   7.486  0.60 31.16      B    N
ATOM   3789  C   ARG B  81      -3.115  34.616  -0.178  1.00 21.97      B    C
ATOM   3790  O   ARG B  81      -3.560  33.632  -0.761  1.00 21.68      B    O
ATOM   3791  N   VAL B  82      -2.029  35.286  -0.559  1.00 20.91      B    N
ATOM   3792  CA  VAL B  82      -1.224  34.884  -1.679  1.00 21.03      B    C
ATOM   3793  CB  VAL B  82      -0.126  35.943  -1.952  1.00 21.89      B    C
ATOM   3794  CG1 VAL B  82       0.869  35.435  -2.906  1.00 22.93      B    C
ATOM   3795  CG2 VAL B  82      -0.734  37.243  -2.483  1.00 21.44      B    C
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ATOM	3796	C	VAL	B	82	-0.583	33.532	-1.371	1.00	20.69	B	C
ATOM	3797	O	VAL	B	82	-0.235	33.255	-0.221	1.00	19.36	B	O
ATOM	3798	N	GLY	B	83	-0.469	32.694	-2.389	1.00	19.91	B	N
ATOM	3799	CA	GLY	B	83	0.382	31.525	-2.331	1.00	20.16	B	C
ATOM	3800	C	GLY	B	83	-0.236	30.295	-2.955	1.00	20.11	B	C
ATOM	3801	O	GLY	B	83	-1.416	30.328	-3.319	1.00	20.36	B	O
ATOM	3802	OXT	GLY	B	83	0.468	29.294	-3.104	1.00	18.79	B	O